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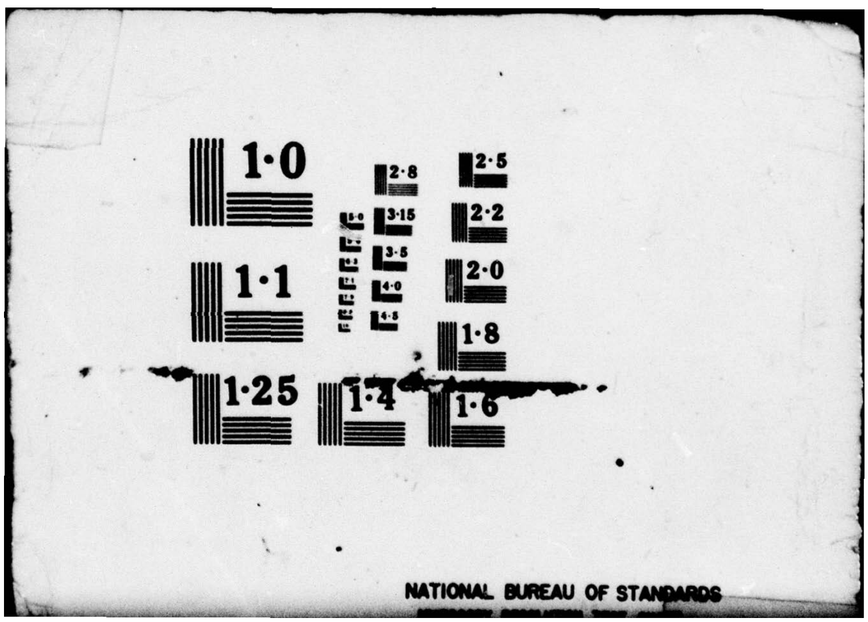
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REVIEW OF TOXIC SPILL MODELING

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This study is a literature survey which identifies existing mathematical models available for the description of toxic spills into waterways. Advantages and disadvantages of numerous models are discussed. Emphasis is placed on model coefficients because these are very difficult to define. Guidelines are presented for coefficient selection. This selection must consider such parameters → over

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as river bends, varying channel geometries, stratified flows and oscillating flows. The interactions of convective transport, turbulent mixing, chemical reactions and other processes are reviewed.

Guidelines are also given for matching the best mathematical model to particular toxic spill scenarios. Modeling technique is discussed to fully describe toxic spills. This literature review provides a useful planning tool for future model development.

PREFACE

This report was prepared by the Department of Civil Engineering, Tulane University, New Orleans, LA 70118 under Contract No. F08635-77-C-0237 with the Engineering and Services Laboratory, Air Force Engineering and Services Center, Tyndall AFB, Florida 32403. The inclusive date of this effort was February 1, 1977 to December 1, 1977.

This technical report has been reviewed by the Information Office and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF SYMBOLS

A = Channel cross-sectional area

B = Channel width

b = Source width in Prych's work

c = Concentration

$\bar{c}$ = Mean concentration

c' = Fluctuation of concentration

c_5 = Threshold c value [Equation (92)]

c_o = Initial concentration

c_p = Specific heat

C_∞ = Completely mixed concentration

D_f = Diffusion factor in stream-tube models [Equation (126)]

D_i = General coefficient

D_L = Longitudinal dispersion coefficient, defined by Equation (19)

$\bar{D}_L$ = Longitudinal dispersion coefficient for equation averaged over one tidel cycle [See Equation (26)]

D_{LS} = Longitudinal dispersion coefficient for slack tide equation [Equation (27)]

D_m = Molecular diffusion coefficient

D_x = Longitudinal coefficient; general, defined initially in Equation (16), but used where other author's coefficient meaning unclear

D_y = Transverse mixing coefficient, defined by Equation (17)

D_z = Vertical dispersion coefficient-similar to e_z, but in various models may include other features.

erf = Error function [See Equation (84)]

e_x = Turbulent diffusion coefficient in x-direction [Equation (8)]

e_y = Turbulent diffusion coefficient in y-direction [Equation (9)]

e_z = Turbulent diffusion ceofficient in z-direction [Equation (10)]

$F_1 = F_1(t)$ = Exponential terms defined in Equation (119)

$F_2 = F_2(t)$ = Exponential terms defined in Equation (120)

$F_3 = F_3(t)$ = Error function terms defined in Equation (123)

f = Darcy-Weisbach friction factor

g = Acceleration due to gravity

h = Channel depth

k_1 = Decay coefficient (same as λ)

k_2 = Decomposition coefficient [Equation (91)]

k_3 = Generation coefficient [Equation (92)]

K_1 = Coefficient in Equation (73) = D_y/hu; also separate definition in Equation (98)

K_e = Surface heat exchange coefficient

K_2 = Coefficient in Equation (98)

L = Distance from streamline of maximum velocity to most distant bank [Equations (67) and (71)]

L_n = Distance to point where longitudinal dispersion is negligible in effect [Equation (89)]

L_o = Total length of estuary

L_* = Half of channel width = $B/2$

M = Total volume of material released = $C_o V_o$

M_b = Dimensionless source strength, Equation (50)

M_d = Dimensionless source strength, Equation (51)

m_x = Metric coefficient, Equation (28) and Figure 1

m_y = Metric coefficient, Equation (28) and Figure 1

n = Manning's roughness coefficient

Q_f = Freshwater inflow

Q_m = Flow rate of discharged material

Q_o = Rate of release of material

q_c = Cumulative discharge in channel [defined in Equation (30)]

r_2, r_3 = Substances decomposed and generated, respectively, per unit volume per unit time

R = Hydraulic radius

R_c = Radius of curvature of bend

R_i = Richardson number [Equation (56)]

r = Function in Equation (52) from Prych's work

S = Salinity

S_o = Reference salinity

T = Temperature; also tidal period

T_c = Cross-sectional mixing time

T' = T/T_c

T_{mix_1} = Time for complete mixing across section [Equation (72)]

T_t = Time scale for horizontal mixing

T_v' = Time scale for vertical mixing

t = Time

U_f = Freshwater velocity

U_{max} = Maximum tidal velocity

u = Velocity in x direction

$\bar{u}$ = Mean velocity in x direction

u' = Fluctuation of x-direction velocity

u_* = Friction (shear) velocity

v = Velocity in y direction

$\bar{v}$ = Mean velocity in y direction

v' = Fluctuation of y - direction velocity

V_o = Volume of released material

w = Velocity in z direction

$\bar{w}$ = Mean velocity in z direction

w' = Fluctuation of z-direction velocity

W_1 = Term defined in Equation (107)

u_o = Maximum cross-section velocity at estuary mouth

u_x, u_y, u_z = Velocity components in three axial directions in natural coordinate system [Equation (28)]

U_t = Maximum tidal velocity

W_2 = Function defined in Equation (145)

x = Longitudinal coordinate direction

x_c = Crossing distance

x_L = Distance to application of 1-D equation

x_m = Mixing distance

y = Transverse coordinate direction

z = Vertical coordinate direction

α = Coefficient defined in Equations (24) and (32) = D_i/hu_*

β_J = Coefficient in Jain's D_L Equation. [Equation (41)]

β_L = Coefficient in Liu's D_L Equation. [Equation (42)]

Γ_y, Γ_z = Transverse, vertical velocity gradients [Equation (147)]

δ = Phase lag

ΔV = Dimensionless excess variance in Prych's work (Figure 2)

ρ = Mass density

ρ_a = Ambient density

$\Delta\rho$ = Density difference

λ = Decay rate

ϕ = Function defined in Equation (149)

ΣS = Sum of all sources and sinks

$\sigma^2(t)$ = Variance of particle distribution

$\sigma^2(x)$ = Lateral variance of concentration profile

τ_o = Bed shear stress

Ω = $(U_f^2 + 4\lambda D_{LS})^{1/2}$ [Equation (140)]

ω = Frequency

SECTION I

OBJECTIVES

PURPOSE OF STUDY

The Air Force, as do many industries, transports, stores, and uses a number of materials which might be toxic to elements of aquatic environments if released to a water body. While such discharges do not occur routinely, there is always some small possibility of an accidental spill of such material.

The current study is therefore aimed at identifying the state of existing knowledge which might be applied to this problem, as well as shortcomings in existing methods. This report will present findings from a preliminary investigational analysis of the prospects for developing a catastrophic spill toxic pollutant model for the general case. Required data inputs will be defined, and influences of local features will be specified. The three-dimensional convection diffusion equation will be presented as modified by the method of images to account for finite source size and finite confining boundaries. Standard means of including reaction terms in the diffusion equation will be reported, with comments on applicability to hydrazine and similar materials.

The interaction of convective transport, turbulent mixing, chemical reactions, and other processes will be reviewed, with examples shown. The information gathered and reported herein will be condensed into a set of recommendations for selection of all input parameters, selection of modeling technique and strategy, and modifications required to fully describe toxic spills of hydrazine or other such materials.

CHARACTERISTICS OF HYDRAZINE

The material of most interest is hydrazine, although the techniques reported here can be applied to any toxic material. It is pertinent, however, to review the physical characteristics of hydrazine to assure that all pertinent features are ultimately included in the final model.

Much has been written about the properties of anhydrous hydrazine (referred to hereafter as simply hydrazine) elsewhere (1)*. Only a few aspects needed for the current discussion will be presented here. Hydrazine is a liquid at ordinary temperatures, is highly reactive chemically, is combustible, and is miscible with water. It displays a marked tendency to absorb oxygen and carbon dioxide from the air. The Air Force currently has underway an extensive program to determine its chemical behavior in the water systems (2).

The density of the liquid may be its single most important property with respect to mixing characteristics in a turbulent field. Walton and Hilgert (3) have suggested the following equation to represent the density.

$$\rho = 1.0253(1-0.00085T) \tag{1}$$

in which ρ = mass density, g/cm^3

T = temperature, ^oC

Table 1 shows values calculated based on Equation (1), along with corresponding densities for water at the same temperatures.

---

*From this point on, it should be understood that numbers appearing in parentheses refer to the references, unless otherwise noted.

TABLE 1. DENSITY OF LIQUID HYDRAZINE

(^{o}C)	ρ, g/cm^3 Hydrazine	ρ, g/cm^3 Water (fresh)
0	1.0253	0.9998
5	1.0209	0.99996
10	1.0166	0.9997
15	1.0122	0.9991
20	1.0079	0.9982
25	1.0035	0.99705
35	0.9948	0.9940
50	0.9817	0.9880

It is important to note that until temperatures above 35^{o}C are reached, hydrazine is more dense than water at the same temperature. In fact, at the lower temperatures, hydrazine densities begin to approach those of highly saline water, close to the density of sea water. The exact density difference between hydrazine and the receiving water body will, of course, depend on the temperatures of the two liquids (which may not be the same) and the characteristics of the receiving water body. If the receiving water body is highly saline, approaching that of sea water, hydrazine will be lighter than the receiving water body. On the other hand, hydrazine will usually be heavier than most fresh waters. Due to stratification existing in many receiving water bodies, the depth of the release may be very important in defining the relative density of hydrazine and the surrounding water.

Section III will deal with the known effects of these density differences. It is clear, however, that in most cases density differences existing between hydrazine and the receiving water will play a major role in the behavior and movement of the hydrazine.

TYPES OF SPILLS ANTICIPATED

For the purpose of the current review, essentially any means by which

the hydrazine or other material would enter a water body is included. The spill can be considered as occurring over any time from instantaneous (the entire quantity is dumped at one time) to continuous (discharge continues long enough for a steady state to be reached in the receiving water). The discharge will usually last a finite time, either until all available material has been spilled or until the problem is found and stopped. It will be seen that the size of the water volume through which the spill enters the water body may range from a point (such as a defined pipe exit) to a volume source (such as might occur if a truck accident occurred, spilling the material into the water over a larger area).

This all simply means that spills as discussed here include those from trucking accidents, tank ruptures draining through storm drains and then to water, or any other accidental introduction of material into a receiving water body.

OUTLINE OF WORK

The work to be accomplished will consist of developing the basic equations, reviewing coefficient values, defining basic means of solving the equations, reviewing available models, illustrating results from some of the models, and presenting recommendations for future work. The work is intended to provide a base for future selection and use of toxic spill models for the Air Force.

It will be seen that an understanding of the physical behavior of an effluent is important in selection and use of a given model. Of equal importance are the coefficients used in the models. Emphasis will be placed on the definition of these coefficients and their physical interpretation.

SECTION II

DEVELOPMENT OF DIFFUSION EQUATIONS

GENERAL COMMENTS

This section outlines the basic diffusion equations to be used in varying circumstances. It will be seen that all such equations germinate from the same basic equations, with various simplifying assumptions made to arrive at reduced forms. Each simplifying assumption has the effect of omitting one or more physical processes from the equation, thereby possibly reducing model predictability.

If empirical coefficients are introduced into the equation (as they are in the diffusion equations) then these omitted terms effectively become absorbed by these coefficients. Thus, it may be possible, by judicious selection of the coefficients, to make acceptable predictions. However, the failure to understand the effects of simplifying assumptions (usually a form of averaging) on coefficients can lead to very erroneous results. The technical literature is full of papers, predictions, and data fittings which fail to recognize this. Therefore, the current report will emphasize a consistent representation of the diffusion, with definition of and distinction between the numerous coefficients. This is essential, as the first step in proper application of a model is correct selection of empirical coefficients as a function of the existing circunstances. Impressive mathematical equations have no value without proper understanding and ability to properly specify parameters.

AVAILABLE WORK AND METHODOLOGIES

Much of the technical literature shows or discusses the development of the basic diffusion equations. It is the intention here to show the basic approaches which are available and then to present a simple view of the development by one method only. The reader will then be referred to a number of possible references for more depth.

The two major approaches to equation development for turbulent diffusion are the Fickian diffusion model and the description of the basic turbulent process by the theory of diffusion by continuous motion. Fick proposed that the molecular diffusion of matter could be expressed in the same manner as the conduction of heat or electricity in a conducting body, as used by Fourier and Ohm, respectively, in their work. This can be stated as making the rate of diffusion in any direction directly proportional to the concentration gradient in that direction. Mathematically, this becomes

diffusion transport rate in x_i direction

$$= -K_D \frac{\partial c}{\partial x_i} \tag{2}$$

in which K_D = diffusion coefficient describing the mechanism (s) leading to the diffusion

x_i = coordinate direction (typically x, y, or z)

Fick proposed this as a means of describing molecular diffusion. Subsequent work has proceeded by expressing the transport due to fluid turbulence as also being proportional to the local concentration gradient. This is a simplification which treats the turbulence in a gross manner as a phenomenon whose effects can be lumped into a single coefficient.

The theory of diffusion by continuous movements was first articulated in an intuitive fashion by Taylor (4) and has been followed up by Batchelor (5), Batchelor and Townsend (6), and Taylor himself (7). This theory attempts to give a kinematic description of turbulent diffusion based on the actual properties of the turbulence. The theory was originally presented for the case of one dimensional dispersion in a turbulence field which is spatially homogeneous and stationary (unvarying) with time. Fickian theory is cast in an Eulerian framework where the frame of reference is fixed and motion is viewed relative to that fixed framework. The statistical (continuous movement) theory, however, is developed in the Lagrangian framework, where discrete fluid particles are followed as they move through the flow field, thereby creating a moving coordinate system with each particle followed.

Reviews of the two approaches are given elsewhere, and the reader is especially referred to works by Fischer (8), Sayre (9), Sayre and Chang (10), Holley (11), and Slade (12). Further details will also be evident in the ensuing sections.

CONVECTION-DIFFUSION EQUATION

The theoretical approach to the diffusion problem is based on the principle of conservation of mass. Any material, pollutant or otherwise, of interest is subject to the same conservation laws. Chang (13) and Holley (11) both outline the initial relationship involving convection and molecular diffusion, and their ideas will be used here.

If a stationary control volume is established in the flow of a mixture of the basic fluid and one or more constituents, the statement of conservation of mass for a marked fluid (fluid constituent of interest) is

$$\left\{\begin{array}{l}\text{Net mass}\\ \text{flux entering}\\ \text{control volume}\end{array}\right\} + \left\{\begin{array}{l}\text{Net rate of production}\\ \text{of mass due to internal}\\ \text{sources and sinks in}\\ \text{control volume}\end{array}\right\} = \begin{array}{l}\text{Time rate of}\\ \text{accumulation of mass}\\ \text{inside control}\\ \text{volume}\end{array} \qquad (3)$$

The mass here refers to the fluid constituent being observed, whether that be BOD, temperature, sediment particles, or other materials. The net mass flux enters the control volume by convection (velocities in the fluid) and molecular diffusion, assumed to follow a Fickian law as in Equation (2). Internal sources and sinks may include deposition, chemical or biological reactions, attenuation of solar radiation, radioactive decay, or other processes.

If the constituent of interest has the same density as the ambient fluid, the convective diffusion equation for molecular diffusion can be written in Cartesian coordinates as

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = D_m\left[\frac{\partial}{\partial x}\frac{\partial c}{\partial x} + \frac{\partial}{\partial y}\frac{\partial c}{\partial y} + \frac{\partial}{\partial z}\frac{\partial c}{\partial z}\right] + \sum S \quad (4)$$

in which

c = concentration of marked constituent or fluid

t = time

x,y,z = Cartesian coordinates

u,v,w = velocity components in x,y, and z directions, respectively

D_m = molecular diffusion coefficient

$\sum S$ = sum of all internal sources and sinks.

1. Turbulent Diffusion - In a turbulent flow field, velocities and concentrations are fluctuating with time. Reynolds first introduced the concept of treating the instantaneous values as the sum of the time-mean value and a fluctuation from the mean, or

$$\begin{aligned} u &= \overline{u} + u' \\ v &= \overline{v} + v' \\ w &= \overline{w} + w' \\ c &= \overline{c} + c' \end{aligned} \qquad (5)$$

in which the overbar implies values averaged over time and the primes indicate the instantaneous fluctuation from the mean.

If these expressions in Equation (5) are inserted into Equation (4) after manipulation, one obtains

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z} = D_m\left[\frac{\partial}{\partial x}\left(\frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{\partial \bar{c}}{\partial z}\right)\right]$$

$$- \frac{\partial}{\partial x}(\overline{u'c'}) - \frac{\partial}{\partial y}(\overline{v'c'}) - \frac{\partial}{\partial z}(\overline{w'c'}) + \Sigma S \qquad (6)$$

The left hand side of Equation (6) can be written using the equation of conservation of mass for an incompressible fluid so that the three convective terms become

$$\frac{\partial}{\partial x}(\bar{u}\,\bar{c}) + \frac{\partial}{\partial y}(\bar{v}\,\bar{c}) + \frac{\partial}{\partial z}(\bar{w}\,\bar{c}) \qquad (7)$$

The terms of interest in Equation (6) are the time-averaged cross products, such as $\overline{u'c'}$. These terms represent the volume flux per unit area due to fluid turbulence and the resulting transfer of material. It is in treatment of this term that the two methodologies (Fickian model and diffusions by continuous movements) already mentioned can be brought to bear.

2. Fickian approach - Here an exact analogy is made to molecular diffusion, as in Equation (2). Specifically, this becomes here

$$\overline{u'c'} = -e_x \frac{\partial \bar{c}}{\partial x} \qquad (8)$$

$$\overline{v'c'} = -e_y \frac{\partial \bar{c}}{\partial y} \qquad (9)$$

$$\overline{w'c'} = -e_z \frac{\partial \bar{c}}{\partial z} \qquad (10)$$

in which e_x, e_y, e_z = turbulent diffusion coefficients in x, y, and z directions.

Insertion of Equation (8-10) into Equation (6) yields

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial y} + \bar{w}\frac{\partial \bar{c}}{\partial z} = \left(D_m + e_x\right)\frac{\partial}{\partial x}\left(\frac{\partial \bar{c}}{\partial x}\right) + \left(D_m + e_y\right)\frac{\partial}{\partial y}\left(\frac{\partial \bar{c}}{\partial y}\right) + \left(D_m + e_z\right)\frac{\partial}{\partial z}\left(\frac{\partial \bar{c}}{\partial z}\right) + \Sigma S \tag{11}$$

Again, the left hand side could be rewritten as in Equation (7). Equation (11) contains the assumption that molecular and turbulent diffusion are independent processes and thus additive, as indicated by terms of the form ($D_m + e_x$). Mickelsen (14) made and justified this assumption. As noted by Sayre and Chang (10), however, it is really only of academic interest in open channel flows, as the turbulent diffusion coefficients are typically several orders of magnitude greater than D_m. For this reason, D_m will be neglected in subsequent presentations of the equation.

The assumptions made in Equation (10), as shown in Equations (8-10), are rather sweeping. Sayre and Chang (10) noted that experimental evidence from a number of sources implies that lateral diffusion is much better represented by the Fickian model than is longitudinal dispersion (as represented by the one-dimensional form of Equation (11), with transport only in the x-direction).

Most workers have found that, despite its theoretical shortcomings, the Fickian model provides a resonable starting point and an approximate kinematic description of diffusion in open channels. It is especially limited by the nature of the coefficients, which attempt to incorporate

many complex influences into a very simple format. The theory itself provides little insight into the actual values of the diffusion coefficients as they are related to the important flow features.

3. Diffusion by Continuous Movements - Taylor (4) introduced a theory which has shed light on diffusion and dispersion processes. He considered dispersion in one direction (say x) in a turbulence field which is both homogeneous and stationary and proved the following relationship for spreading out of particles beginning at x = o for t = o.

$$\sigma^2(t) = 2\,\overline{u'^2} \int_0^t (t - \tau) R(\tau)\, d\tau \qquad (12)$$

in which

$\sigma^2(t)$ = variance of particle distribution in x-direction at time t

$\overline{u'^2}$ = mean of squared instantaneous velocity fluctuations

$R(\tau) = \overline{u'(t)u'(t+\tau)} / \overline{u'^2}$

= Lagrangian auto correlation function, which correlates values of u' from one time to the next instant.

$R(\tau)$ is difficult to determine, but it approaches 1 for small τ and o for large τ. With this knowledge, it can be shown that for small times

$$\sigma^2(t) = \overline{u'^2}\, t^2 \qquad (13)$$

and for large times

$$\sigma^2(t) = 2\,\overline{u'^2}\, t\, T_L \qquad (14)$$

in which T_L = the Lagrangian integral time scale. It can be found that Equation (14) has the identical form of the variance for longitudinal dispersion from the Fickian model.

Since Equation (12) was originally derived for homogeneous turbulence fields, it may appear inapplicable to open channel flows, where statistical properties are known to vary with the distance from the boundary. However, Sayre and Chang (10) review work by Orlob (15, 16) and Batchelor and Townsend (6) and note that Equation (12) applies, under conditions of uniform flow, to lateral diffusion and longitudinal dispersion in planes parallel to the bed in wide channels, and that Equation (14) applies to longitudinal dispersion in any uniform channel. They note that this gives very strong theoretical support to the applicability of the Fickian diffusion model to longitudnal dispersion in open channels for sufficiently large dispersion times. Evaluation of what constitutes a "sufficiently" large time will be discussed in Section III.

4. Summary on Convective-Diffusion Equation - The preceding sections have attempted to show the development of the convective-diffusion equation for three dimensions, as in Equation (11). The use of the Fickian model analogy to molecular diffusion Equations (8-10) is important to note. Because of the ill-defined nature of the coefficients in these equations a better understanding of their variation and the physical patameters influencing them is essential. The current state of knowledge in this area will be reviewed here.

Fischer (8) notes that there are limitations to use of a gradient-type coefficient for turbulent transport [(as in Equations (2) and (8-10)]. In the oceans, for example, particles are usually separated by a distance smaller than the largest scale of turbulent motions; thus, the farther apart particles move, the faster they tend to separate, leading to the well-known four-thirds law, shown in Equation (33). Fischer notes, however, that in open-channel flows the turbulence scale is limited by the depth,

and it is possible that a group of tracer particles may be spread over distances larger than the largest scale of turbulence, thus making the concept of a gradient-type mixing coefficient reasonable.

In summary, despite some theoretical shortcomings, Equation (11) gives a rational form for describing diffusion processes, and it will be used for further work in this report.

SPATIAL AVERAGING OF EQUATIONS

Equation (11) is valid at any point in the flow field. Ideally, solution of the equation would include consideration of the individual components at each point in the flow field. Inadequate knowledge of the flow processes limits the ability to obtain such a solution. One should recall Equation (11) already includes one simplification, represented by replacement of turbulent fluctuation terms by Equations (8-10). To obtain a solution, other simplifications may be necessary. In addition, certain physical situations exist in which it appears acceptable to treat something less than three dimensions. For example, if the pollutant seems likely to be well-mixed vertically in the water body, it would appear practical to consider a two-dimensional model. However, each simplification introduced into the equations also introduces more physical effects which must be described by the free parameters in the equation, i.e., the diffusion coeffiecients. In discussing the two-dimensional equation, Pritchard (17) notes that "The greater the detail provided by the model with respect to variations in velocity in time and space, the less significant are the horizontal eddy diffusion terms ..." (page 17). It is important to understand which things are included in each coefficient, and therefore a brief review of the effects of spatial averaging will be presented here.

1. Depth Averaging: Two Dimensional Equation - In most open channel (river or estuary) situations, the depth is much less than the width, and it may appear reasonable to assume that the tracer material is mixed fully throughout the vertical structure of the water body. This assumption can be utilized to integrate Equation (11) over the depth, h, of the water body, thereby reducing the equation to a two-dimensional equation. Values for all the parameters will then be depth-averaged values. Integration with depth will also eliminate the vertical diffusion term, e_z. As shown by Holley, et al (18), Equation (11) can be integrated vertically to yield

$$h\left(\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y}\right) = \frac{\partial}{\partial x}\left(hD_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(h\,D_y\frac{\partial c}{\partial y}\right) \tag{15}$$

in which all values are depth-averages, and D_x and D_y are defined by

$$-\overline{D}_x \frac{\partial c}{\partial x} = \overline{u'c'} - \overline{e}_x \frac{\partial \overline{c}}{\partial x} \tag{16}$$

$$-\overline{D}_y \frac{\partial c}{\partial y} = \overline{v'c'} - \overline{e}_y \frac{\partial \overline{c}}{\partial y} \tag{17}$$

u', v', c' = deviation from depth average value of u, v, and c respectively

(Overbars imply depth average, and have been omitted in Equation (15)

It can be seen from Equations (15) and (16) that the longitudinal coefficient, D_x, now includes mixing due to both turbulent diffusion (the e_x term) and differential advection due to vertical variation of longitudinal velocity and concentration. It has been shown that the turbulent diffusion term is negligible in this instance. Similarly, D_y includes diffusion and differential lateral advection. The relative magnitudes of these terms depends on the physical setup. However, bends, overbanks, or other configurations which create transverse flows in channels may make the

advective term become very large. Holley, et al (18) and Krishnappan and Lau (19) both note that spreading due to transverse velocities can easily exceed spreading due to turbulent diffusion. It is important to recall these approximations in selecting coefficient values.

2. Width Averaging - One-Dimensional Equation - If Equation (15) is further integrated across the entire channel width, it yields

$$hB \left(\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} \right) = \frac{\partial}{\partial x} \left(BhD_L \frac{\partial c}{\partial x} \right) \tag{18}$$

in which all values are cross-sectional averages and D_L = longitudinal dispersion coefficient.

This equation is often called the longitudinal dispersion equation or the one-dimensional dispersion equation. The coefficient D_L is defined by

$$-D_L \frac{\partial \bar{c}}{\partial x} = \overline{u''c''} - \bar{D}_x \frac{\partial \bar{c}}{\partial x} \tag{19}$$

in which u'' = variation of velocity from cross-sectional mean

c'' = variation of concentration from cross-sectional mean.

Overbars imply an average over the stream cross-section. Again, overbars are omitted in Equation (18).

The coefficient D_L now contains not only the elements in D_x, but, in addition, the spreading out of material due to differential velocities (and concentration) across the stream. Fischer (20,21) has noted that in rivers this latter contribution is by far the largest of the components included in D_L. A review of the developments shows that D_L now includes the effects of the following physical processes:

Molecular diffusion (D_m)

Turbulent diffusion (e_x)

Vertical variation of velocity and concentration.

Lateral variation of velocity and concentration.

Typically, in open channels, the increase from one mechanism to the next is at least one order of magnitude. For example, the coefficient contribution due to vertical variation is at least one order of magnitude greater than turbulent diffusion in the x-direction. In some estuarine situations, however, it will be shown that the vertical variation will be more important than lateral variations.

The relationship between the longitudinal coefficient and the lateral diffusion coefficient has been reviewed by Fischer (20), who obtained the following equation.

$$D_L = -\frac{1}{A}\int_0^B u''(y)h(y)\left[\int_0^y \frac{1}{D_y h(y)}\left\{\int_0^y \int_0^{h(y)} u''(y)dz \quad dy\right\}dy\right]dy \tag{20}$$

in which

h(y) = local depth

A = cross-sectional area of flow

u"(y) = local deviation of longitudinal velocity from cross-sectional mean.

Note that Equation (20) not only indicates a strong contribution due to lateral variation of the longitudinal velocity, but also shows the limiting effect of lateral diffusion, as given by D_y. Higher degrees of lateral diffusion tend to slow longitudinal spreading, as material which is moved ahead of particles in adjacent flow paths would tend to establish a high lateral gradient. This high gradient, coupled with high D_y values, would spread the material laterally and tend to lessen the longitudinal spreading out of the particles. Fischer (21) has used Equation(20) as a basis for evaluating longitudinal coefficients based on field information.

3. Partial Averaging: Velocities - Frequently, the diffusion equation is written using velocities which are average values over the cross-sectional area. In Addition, the lateral and vertical velocity components, v and w respectively, are often neglected. Even if the spatial average of one or both of these is zero, the value (s) is individual points will be nonzero.

Consider first the neglect of v and w. Referring to Equation (11) assuming v = w = o would result in dropping the following terms:

$$v \frac{\partial c}{\partial y} \text{ and } w \frac{\partial c}{\partial z}$$

Further, notice the similarity of the form of these terms to the diffusion terms on the right hand side of the equation. It can logically be expected that the contribution to mixing due to the actual transverse velocity field, v(x,y,z,t) will be absorbed in the D_y term when v is neglected. A similar statement holds for absorption of vertical mixing into the D_z term when w is assumed to be equal zero. Notice, however, that the replacement can never be exact unless D_y and D_z are made to vary with x,y,z and t so as to duplicate the effects of v and w. Typically, this is not done; instead, modified values for D_y and D_z are employed which purport to encompass these effects.

Similar statements can be made concerning the use of a spatial average value of the longitudinal velocity, u, at each point. Use of $\bar{u}$ at each point means that the expression in Equation (11) at any individual point in the flow field has neglected a term, $u' \frac{\partial c}{\partial x}$. This term can be either positive or negative, depending on the value of u' at that point in the section. For any given point in the flow field, it would be possible to compute values for other terms, especially the advective terms, and determine the relative magnitude of the neglected term. However, the full three-

31

dimensional equation result cannot be compared directly to that using an average $\bar{u}$ except by a full solution using finite element or finite difference techniques. This is because the integrated mixing history of a parcel of material is a function of all the velocities to which it is exposed.

Whatever view is used, however, neglect of u' terms loses some detail from model description of the mixing process. These processes then get lumped into the D_x term in Equation (11), also a function of $\frac{\partial c}{\partial x}$. This expression is then similar to D_L, the longitudinal dispersion coefficient seen in Equation (18). In fact it can be shown by integration of Equation (11) with $\bar{u}$ instead of u that D_x is numerically equal to D_L for that use.

4. Partial Averaging: Depths - Another very common simplification is the assumption of a constant depth across the channel section. This effect can be reviewed by looking at several of the preceding equations as well as by considering the physical implications. It should be noted that there is a relationship between the local depth and the velocity. Sayre and Caro-Cordero (22) have noted that a preliminary review of some available data indicates that

$$\frac{q}{\bar{q}} = \left(\frac{h}{\bar{h}}\right)^{5/3} \tag{21}$$

in which q = discharge per unit width at any location across the section where the local depth is h

$\bar{q}$ = cross-sectional average of the q

$\bar{h}$ = average depth at the cross-section

Regardless of whether Equation (21) provides the final form of the u versus h relationahip, it is clear that neglect of depth variations can lead to problems similar to assuming a single, constant value of u.

Equation (11), as noted, can be written in a form including the conservation of mass relationship. For the current discussion, the conservation of mass equation will be considered separately, as shown in Equation (22).

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \tag{22}$$

Integration of this equation over the depth in a steady flow (implying w = 0 at both the stream bed and the water surface) yields

$$\frac{\partial(uh)}{\partial x} + \frac{\partial(vh)}{\partial y} = 0$$

Here, u and v are now depth-averaged values. Further integration, as shown by Holley (23), with respect to y results in an expression for the lateral velocity, v.

$$v = -\frac{1}{h} \frac{\partial}{\partial x} \int_{s}^{y} uhdy \tag{23}$$

where s is a point in a streamline. Holley (23) states that to study diffusion data, the value of the transverse velocity of interest is the one which describes the movement of marked fluid particles relative to the streamline through the point of release. Therefore, s should be located on that streamline. A look at Equation (23) shows that if h and u have been assumed constant, then the value of v will be zero. This would be so because physically no transfer of material from one stream tube to another could possibly take place if neither velocity nor depth changed, if stream tube widths remain unchanged. Physically, then, assumption of a constant depth along with a constant velocity has the effect of eliminating detail of the transverse velocity field. This would be similar to the neglect of terms such as $v\frac{\partial c}{\partial y}$ from Equation (11), which results in changes in the lateral coefficient values to accommodate the loss of description of advective motion.

Fischer (24,25) notes that some of the largest contributions to values for D_L in estuaries appear to be the lateral currents created by depth variations. The water tends to move up over the shallower, overbank regions as the tide rises and to move back toward the main channel as the tide falls.

Holley, et al (18) numerically experimented to compare mixing behavior in rectangular and trapezoidal channels, using a finite-difference model. Discharges into the shallower water near the shore always displayed higher near shore concentrations than the same discharge into a rectangular channel of constant depth. What is happening here is that less water is available for dilution in these shallower regions. Hence, any solution which replaced the channel with some equivalent rectangular channel might underestimate these near shore concentrations. Unfortunately, it is frequently these very concentrations which are most critical in many biological systems.

In summary, it can be stated that use of a constant depth may lead to a number of possible misrepresentations of the actual physical behavior. These misrepresentations will cause the values of the coefficients to change from the standard values if an attempt is made to reproduce data. If no data exists, the possibility for erroneous predictions exists. In addition, coupling an assumed constant depth with an assumed constant velocity results in further failure to adequately describe the advective motion.

5. Partial Averaging: Coefficients - A final area in which constant values are often assumed is in the coefficients chosen to represent a given cross section reach. It will be discussed further in the next section that a basic form for the diffusion coefficients is

$$D_1 = \alpha h u \tag{24}$$

in which D_1 = coefficient of interest
α = coefficient

This is usually applied in an overall sense, choosing average h and u values over a reach. However, as noted by Holley, et al (18) and Eheart (26), there is some logic to the possibility that, for example, the transverse mixing coefficient might vary as a function of the local values of h and u at any given point. If this were true, then assumption of constant coefficients and removal from the derivations would omit some terms. For example, consider the lateral diffusion term from Equation (11),, using Equation (24) to describe D_y

$$\frac{\partial}{\partial y}\left(D_y \frac{\partial c}{\partial y}\right) = D_y \frac{\partial^2 c}{\partial y^2} + \frac{\partial c}{\partial y}\left(h \frac{\partial u}{\partial y} + u \frac{\partial h}{\partial y}\right) \qquad (25)$$

The first term on the right hand side in Equation (26) represents a common way of replacing the general expression on the left hand side. Note that if the coefficient were a function of local u and h values, then the other right hand side terms would be neglected by assuming a single, constant D_y value. In that case, the D_y value would again be modified by attempting to incorporate those neglected mechanisms.

The current state of knowledge is not such as to enable a definitive statement of how D_y and the other coefficients vary. Indeed, over longer reaches, Krishnappan and Lau (19) and Chang (13) indicate that use of single coefficient values may be adequate, although in local regions in bends this may not be so. As better knowledge becomes available, it may be possible to better decide the influence of the neglected terms from Equation (25).

It is important to observe that similar considerations can be made if u and h are varying in time, meaning that the coefficient value is not a constant. Any model which assumes a time-invariant value for any or all coefficients is then trying to lump all this neglected behavior into the coefficients.

TIME AVERAGING OF THE EQUATION

One form of time averaging has already been discussed in considering the short-term turbulent fluctuations by the Reynolds method [(see Equations (5)-(7)] and the replacement of the covariance terms by the terms in Equation (8). Of interest now is the use of longer term averaging, for example, over the period of a tidal cycle. Actually, any time an unsteady flow is treated as steady, the equation is effectively averaged. As the tidal cycle usually represents the most extreme unsteadiness of concern in water quality problems, emphasis here will be placed on that area. However, river systems exhibit unsteady flows as well, and those which have dams controlling flow downstream of the site of interest often exhibit flow reversals as well. Therefore, while more has been written about tidal systems, rivers should receive as much attention in future work.

Harleman (27) gives an excellent discussion of the various approaches, and his comments will be briefly summarized here. For this discussion, reference will be made to the one-dimensional, longitudinal dispersion equation written in Equation (18). The term hB (depth times width) will be replaced by A (the cross-sectional area) to make the equation general. The source and sink terms will be omitted, but it should be recognized that they must be included for general use. It is, however, the advective and dispersion terms which are of most interest in defining the averaging problems. The modified version of Equation (18) will be referred to as the real-time equation, since it could be applied to any point in time.

Two approaches both yield models which can be classed as non-tidal advective models, since the advective terms representing tidal velocities have been eliminated. One such approach uses an average over the tidal cycle, while the other deals only with the points in time called slack tide.

Arons and Stommel (28) and Stommel (29) proposed averaging each term of Equation (18) over a tidal period, yielding Equation (26).

$$\frac{\partial \overline{c}}{\partial t} + U_f \frac{\partial \overline{c}}{\partial x} = \frac{1}{\overline{A}} \frac{\partial}{\partial x}(\overline{A}\ \overline{D}_L \frac{\partial \overline{c}}{\partial x}) \qquad 26$$

in which the overbar represents the average value over the tidal period and

U_f = non-tidal advective velocity due to freshwater inflow $= Q_f/A$

Q_f = freshwater inflow.

Note that all mass transfer effects due to the tidal component of the advective velocity, and hence such effects must appear in the time-averaged dispersion term.

Occasionally Equation (26) is rewritten by setting the time derivative equal to zero and then further assuming that the freshwater inflow, $Q_f = \overline{A}\ U_f$, is a constant. This yields a so-called steady state equation, inasmuch as $\overline{C}$ does not change from one tidal period to the next if the boundary conditions for $\overline{C}$ are also constant. This use of the wording steady state occurs in a number of estuary references and can be confusing.

The second non-tidal advective model approach is the slack tide approximation, formulated especially by the Manhattan group led by O'Connor, and exemplified in O'Connor and DiToro (30) and O'Connor (31). Their models apply only to the specific instant of slack tide and not to any intervening time. In many cases data in estuaries are only available at times of slack tide. High water slack refers to the point at which flood tide changes to ebb tide, while low water slack is the reverse. Slack tide is actually that time at which the total velocity (tidal plus freshwater) equals zero, but O'Connor retained the freshwater velocity, Q_f/A. This slack tide yields

$$\frac{\partial C_s}{\partial t} + \frac{Q_f}{A}\frac{\partial C_s}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}\left(AD_{LS}\frac{\partial C_s}{\partial x}\right) \tag{27}$$

in which C_s = concentration at slack tide

A = across-sectional area at slack

D_{LS} = dispersion coefficient

Again, all the advective behavior of tidal action which is neglected from one slacktide to another must be handled in the dispersion term. The three equations [(18), (26) and (27)] attempt to describe the same system, but the three coefficients - D_L for the real time equation, $\bar{D}_L$ for the tidalperiod-average equation, and D_{LS} for the slack tide approximation - all represent somewhat different phenomena. Typically, the latter two coefficients are much larger than D_L as they must encompass such a large amount of neglected tidal advective behavior.

SUMMARY ON AVERAGING EFFECTS

The preceding sections have had the goal of outlining a way of thinking about coefficients and their meaning as well as equations in which they appear. Each time one or more terms of the equation is averaged in space or time, some of the detailed behavior associated with those terms is lost. The only mechanism left for trying to reproduce that neglected portion of the behavior is through the values assigned to the diffusion and dispersion coefficients in the equation. It should be clear, then, that in common uses of the equation the coefficient values are strongly a function of the physical situation at the site and the characteristics of the discharge, as these determine the relative magnitude of the transverse velocities, tidal velocities, or whatever other behavior has been neglected or simplified. Indeed, some cases may actually require more detailed treatment than can be generated solely from the convective-diffusion equation, especially those where initial mixing or density-driven currents exist.

The models can be used for at least two classes of problems. First, the models may be used to predict concentrations where little, if any, prototype verification data exists. In these cases, the physical processes must be reviewed to assure the best choice of coefficients. The second category of problems involves those cases where extensive verification data does exist at the site. In these cases, the problem is one of fitting the equations to data to establish coefficient values. However, the physical mechanisms involved must be fully understood to avoid misuse of these fitted values or extrapolation, to cases where the controlling physical parameters are different. One example is: erroneously used diffusion coefficients obtained from non-buoyant dye releases for predicting the behavior of buoyant discharges. As another example, ambient mixing and hence diffusion coefficient values will vary from one part of a bend to another. With these factors to review in transposing from one flow to another at the same site, it is clear that extreme care is needed in transposing data and coefficients from one site to another.

Specific numerical values will be presented in the discussion on coefficient selection section. The key elements to remember are (1) the coefficients in the diffusion equation encompass many more physical phenomena than just turbulent mixing, and (2) coefficient values for any given case are strongly a function of both the physical system and the equation being used.

USE OF CURVILINEAR COORDINATE SYSTEM

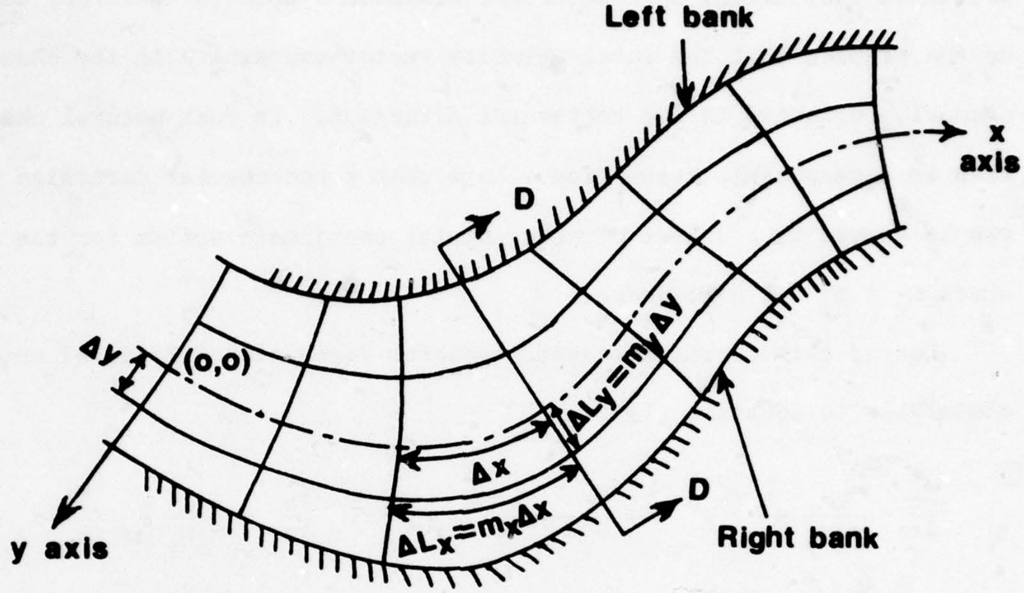
A number of authors have developed the basic diffusion equations in a curvilinear coordinate system rather than the Cartesian system.

The curvilinear coordinate system recognizes the natural channel curvature which almost always exists in natural streams of any length. In addition, even in rather straight channels, irregularities in the channel bottom due to structures, sediment deposition, and the like may yield a nonuniform channel and hence, lead to some of the same transverse velocities of interest in river bends.

From a strictly theoretical point of view, there are some advantages to the use of a curvilinear system. It has to this time been used less widely than the Cartesian and therefore has received less attention in this review. However, it is likely to be utilized widely in the future, and its combination with the use of the cumulative discharge as the independent variable shows real potential for certain classes of problems.

Yotsukura (32) presents a very comprehensive and rigorous derivation of the basic equations. Chang (13) and Fukuoka and Sayre (33) also employed this system, often called the natural coordinate system. The system is composed of three mutually orthogonal sets of coordinate surfaces, called by Yotsukurs (32) the longitudinal, transverse and horizontal coordinate surfaces. The longitudinal and transverse surfaces are vertical, typically curved and nonparallel. The horizontal surfaces are all parallel, horizontal planes. The longitudinal surfaces are usually aligned approximately in the direction of the depth-averaged total velocity vector. The origin and the three coordinate axes - x,y, and z - are shown in Figure 1. (Note that Yotsukura's y and z make this consistent with the current report's notation.

Due to channel curvature and changes in width, metric coefficients m_x and m_y are introduced to correct for differences between the distances measured along any given surface and those measured along the corresponding axes. These are illustrated in Figure 1. The values of m_x and m_y may vary from point to point, being functions of both x and y. Note that m_x=1



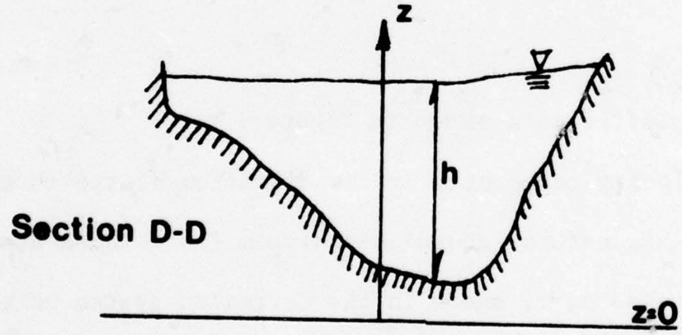


Figure 1. Schematic of Natural Coordinate System

on the x axis and $m_y = 1$ on the y axis. Due to the parallel nature of all horizontal coordinate surfaces, the value of m_z is one everywhere. As Yotsukura (32) notes, this natural coordinate system is therefore based on the premise that the total velocity vector everywhere in the channel is primarily oriented in the horizontal direction. In most natural channels, this is a reasonable assumption. Note that a rectangular Cartesian system can be viewed as a subset of this natural coordinate system for the case where $m_x = m_z = 1$ everywhere.

Use of this coordinate system enables derivation (13, 32) of an equation comparable to Equation (11).

$$\frac{\partial c}{\partial t} + \frac{u_x}{m_x m_y} \frac{\partial}{\partial x}(m_y c) + \frac{u_y}{m_x m_y} \frac{\partial}{\partial y}(m_x c) + u_z \frac{\partial c}{\partial z} = \frac{1}{m_x m_y} \frac{\partial}{\partial x}\left(\frac{m_y}{m_x} e_x \frac{\partial c}{\partial x}\right) + \frac{1}{m_x m_y} \frac{\partial}{\partial y}\left(\frac{m_x}{m_y} e_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(e_z \frac{\partial c}{\partial z}\right) \tag{28}$$

in which

m_x, m_y = metric coefficients shown in Figure 1

u_x, u_y, u_z, = velocity components in the direction of the three axes in the natural coordinate system (note these are not the same as u, v, and w in the Cartesian system unless the channel is straight and uniform)

For comparison, the mass conservation equation for water is written as

$$\frac{\partial}{\partial x}(m_y u_x) + \frac{\partial}{\partial y}(m_x u_y) + m_x m_y \frac{\partial u_z}{\partial z} = 0 \tag{29}$$

Yotsukura (32) notes a major theoretical advantage due to approximate alignment of the natural coordinate axes with the velocity vectors. Theoretical developments beyond the scope of the current paper have defined the diffusion coefficients as a tensor (3 by 3). Hinze (34) and

Dagan (35) note that if only the three principal coefficients (e_x, e_y, and e_z) are to be used, this alignment with the flow field is essential. This is a plus for the use of this system , but current lack of knowledge of the diffusion process and proper selection abd use of equations and coefficients probably masks errors due to failure to satisfy this criterion in standard Cartesian systems.

Yotsukura (32) does an excellent job of providing a rigorous and through development of the equations through the process of depth and then width averaging. A review of this paper is an excellent starting point for understanding the natural coordinate system and the whole process and effects of equation averaging.

USE OF CUMULATIVE DISCHARGE AS INDEPENDENT VARIABLE

An added step has been introduced by Yotsukura (37) and Cobb (36) to further deal with the difficulties associated with varying channel geometry and alignment. They suggest a transformation whereby the transverse coordinate is replaced as an independent variable by the cumulative discharge from the shore to that transverse point in the channel cross section. The transformation can be identified by the relationship (38)

$$q_c = \int_{y_L}^{y} m_y h u_x \, dy \qquad (30)$$

in which q_c = cumulative discharge in channel flowing between coordinates passing through y_L and y

y_L = coordinate of left bank.

The cumulative discharge, q_c, can be used as the independent variable (in place of y) for two-dimensional, steady-state problems. Equation (30) shows that integration over depth has already occured in the definition, hence limiting it to two-dimensional cases. Yotsukura (37) and Sayre (38)

incorporate this into the diffusion equation for steady-state conditions. They first note that in steady-state conditions, the work of Sayre and Chang (10), among others, justifies neglect of the longitudinal dispersion term except near the source. Note that if either the flow or the pollutant input is unsteady, this places a limit on use of this model. In fact, Thomann (39) indicates that variation of the input with any period less than one week requires inclusion of the longitudinal dispersion term in the one dimensional equation. Serious constraints are unlikely with this current model, but the possibility should not be ignored. The two-dimensional version of Equation (29) is written and integrated from y_L to y, including the relationship in Equation (30). The result is substituted into the two-dimensional form of Equation (28) with the longitudinal dispersion term dropped and yield

$$\frac{\partial c}{\partial x} = \frac{\partial}{\partial q_c} \left(m_x h^2 u_x D_y \frac{\partial c}{\partial q_c} \right) \tag{31}$$

If m_x is set equal to one in Equation (31), it becomes identical to the form shown by Yotsukura and Cobb (36), for a straight, uniform channel where $u_z = 0$.

One important factor in use of Equation (31) is that no specific data needs to be provided about the transverse velocities u_y. The cumulative discharge information can be attained by information on longitudinal velocities and channel cross section geometry, both of which are made easier to measure than are transverse velocities.

Use of the natural coordinate system has introduced the metric coefficients m_x and m_y. Some uncertainty exists as to their full significance. However, they probably are not a big problem is use of the approach. Sayre and Yeh(40) report that they found values of m_x ranging from 0.86 to 1.14 in an extremely sharp bend in the Missouri River, indicating that there will usually

be only small differences from unity if the x axis is located in the central part of the channel.

CONCLUSIONS TO SECTION II

The basic form of the convective - diffusion equation, Equation (11), contains all advective terms and diffusion terms. The only averaging which has taken place is over the short time intervals of turbulent fluctuations. However, for mathematical simplicity, other forms of the equation are frequently used which introduce various forms of spatial and/or temporal averaging. Each time such an averaging takes place, one or more terms is effectively dropped from the equation. Practically, this means that the physical effects represented by these terms must be absorbed by the only free parameters in the equation, the coefficients. Basically, the coefficients are required to make up for shortcomings in describing the advective flow fields.

The major items averaged in equation simplification are the longitudinal velocity and the depth of flow. A further simplification occurs if lateral or vertical velocities are neglected, leaving their often substantial influence to be handled by the lateral and vertical coefficients respectively. A knowledge of the averaging steps undertaken to formulate a given model is essential to being able to select coefficients.

Two recent developments offer some an alternative approach to the standard formulation of the diffusion equation. Both may help overcome problems associated with bends in a river. One technique involves writing the equations using the natural coordinate system, which follows the axis of the river. The other technique uses the cumulative discharge (total discharge between the bank and the point of interest) as the independent variable rather than the lateral distance, y. This has been shown to provide a good fit to field data. If accurate information can be provided

on velocity variation within the section, this may prove to be a very useful way to incorporate channel geometry into the equation.

SECTION III

COEFFICIENT SELECTION

INTRODUCTION

Following the discussion of the factors lumped into the various coefficients by equation development procedures, it seems appropriate to review available information on selection of numerical values for those coefficients. The emphasis throughout will be on presenting the basic information, citing references to enable the reader to pursue it in more detail, if desired. Reference will be made on numerous occasions to the developments in Section II on effects of equation averaging on these values. It is essential to read the material in this section with the understanding that the coefficients are strongly functions of the (1) physical situation at the individual site and (2) the equations being employed.

A few comments about terminology are in order. A review of the literature reveals an extradinarily large variety of designations applied to the coefficients. Unfortunately, even now there is no uniformity of the jargon used in the technical literature. This can lead to confusion when reading reports and journal articles. The safest thing to do is to understand fully what equation is being used and understand what advective components are included in the coefficients, thereby bypassing problems of definition.

There is occasionally concern over proper use of the words diffusion and dispersion. Some have suggested that diffusion apply only to the resultant of temporal averaging over the scale of turbulent fluctuations, with dispersion reserved for any results of spatial averaging with depth and/or width. Others use dispersion only to apply to the one-dimensional equation [Equation (18)], while still others call any and all processes

dispersion, which at the very least avoids problems with jargon. Other workers have circumvented the problem by referring to transverse mixing or longitudinal mixing. The tendency in this report will be to use the term mixing along with diffusion for vertical and transverse processes, and dispersion for longitudinal processes where spatial averaging has occurred beyond Equation (11). The key point is the understanding of <u>what the coefficients mean</u>. Then terminology is less of a problem. Still, it is hoped that some consensus will eventually be reached on the terms to be used.

BASIC FORMULAE

There are two main approaches used to express values for the diffusion coefficients. The first of these relates the coefficient to the depth and friction velocity, while the second - the so-called four-thirds law - relates the coefficient to the scale of mixing raised to the four-thirds power. Current practice is to use the former formulation for rivers and estuaries, while the second is used for more open water bodies, such as oceans, lakes, large embayments, and the like. The four-thirds law is often used in atmospheric mixing problems as well. In these large systems, the largest scale of turbulent motion ("eddies") is usually larger than the distance between any two tracer particles of interest. Theoretical development for the two particle separation problem indicates they separate faster the farther apart they are, following something like the four-thirds law (5, 41). The physical phemonenon here can be understood by realizing that as the particles move further apart, larger scale eddies can act to move them apart at an increasing rate.

Due to the concept of relative eddy size, the use of a gradient-type approximation of diffusion, as in Equation (2), has been questioned. However, as Fischer (8) notes, in typical open-channel flows, the scale of turbulence is limited by the channel bottom or the flow depth. He notes that

if the cloud of particles is well distributed over the depth, then the particle cloud may be larger than the largest scale of turbulence, and hence a gradient approximation is reasonable.

1. Friction Velocity Formulation- The basic expression here arose from the theoretical work of Taylor and Elder (42) and takes the form (4)

$$D_i = \alpha h u_* \tag{32}$$

in which D_i = diffusion or dispersion coefficient of interest

α = coefficient

u_* = friction (or shear) velocity

$= \sqrt{\tau_o / \rho}$

Other measures of the depth, such as the hydraulic radius, may be used.

Holley, et al (18) used the mean velocity in the channel instead of u_*. This is not frequently done, but it is worh noting the relationship between U, the mean *velocity*, and u_*. *From any standard* fluid mechanics text, it can be found that

$$\frac{U}{u_*} = \sqrt{\frac{8}{f}} \tag{33}$$

in which f = Darcy-Weisbach friction factor. For cases where incomplete knowledge exists at a given site, Equation (33) might be used to estimate u_* by estimating f and U.

2. Four-thirds Law Form - The basic expression here can be written as

$$D_i = K L_i^{4/3} \tag{34}$$

in which K = a constant, dependent on units used

L_i = scale of plume in direction of interest (i.e., size of plume)

The value of the constant K has been taken as various values, dependent upon the particular data reviewed. However, the data reported by Wiegel (43) indicates that the range of K is about 0.0001 - 0.01 for D_y and a

reasonable value is 0.001, for units of L in feet and D_y in ft^2/sec.

PREVIOUSLY REPORTED COEFFICIENT VALUES

Representative values for the coefficients will be given in the following sections, with emphasis on "standard" values. Then, succeeding sections will review the effects of varying physical features, such as bends, flow unsteadiness, etc. There will be obviously some overlaps, as reported data does not always clarify which physical features are present. This, in fact, is one of the dangers in transposing data from one site to another.

1. Vertical Mixing - Less work has been done on vertical mixing than on transverse and longitudinal, probably because of its lesser importance in many practical open channel problems. However, analytical developments by Elder (42), predict a parabolic variation of the vertical momentum transfer, which is assumed equal to the rate of mass transfer. This parabolic variation has been verified experimentally by Jobson and Sayre (44). The peak value of e_z is about $0.09hu_*$, while the depth-averaged value, as noted by Fischer (8), can be taken as about.

$$e_z = 0.067hu_* \qquad (35)$$

in which e_z = depth-averaged value.

2. Transverse Mixing - Most work on transverse mixing has been done by making measurements, either of the spread of floating particles placed on the surface or by the spread of a dye or other dissolved tracer placed into the flow. Fischer (8) summarizes results tabulated by Prych (45) and Okoye (46) covering a range of reported values. These are reported in Table 2.

TABLE 2. REPORTED VALUES FOR TRANSVERSE MIXING IN OPEN CHANNELS

Type of Experiment	Reference	Location	D_y / hu_*
Floating particles	47	Lab flume	Average 0.16
	48	Lab flume	0.24
	10	Lab flume	0.196-0.264
	49	Lab flume	0.204-0.234
	45	Lab flume	0.167-0.252 (Average of 13 runs = 0.204)
Lab tracer studies	50	Lab flume	0.08
	42	Lab flume	0.16
	10	Lab	0.16-0.179
	51		0.107-0.133
	46		17 runs-avg. = 0.14
	45		13 runs - avg. = 0.135
River tracer studies	52	Columbia River	0.72
	53	Atrisco Feeder Canal	0.24-0.25
	54	Missouri River	0.6

It appears that the coefficient, at least in a straight channel free of extraneous behavior such as transverse velocities, ranges from about 0.2 hu_* at the surface to zero at the stream bed, with a depth-averaged value

$$D_y \approx 0.15hu_* \qquad (36)$$

A glance at the field results shown indicates the large changes in coefficient values which can occur when other factors come into play. Several of these factors will be discussed in succeeding sections.

3. Longitudinal Mixing - It is considerably more difficult to categorize the values to be assigned here once the coefficient D_z is reached. This is due partly to the wide variety of velocity variations

found in natural channels and partly due to the tendency to apply the one- dimensional equation to cases which are not in fact one-dimensional.

For most practical applications, the value of e_x has little significance due to its small value, but if it is assumed (10, 42) that the turbulence is isotropic merely for the sake of an estimate, then e_x is approximately equal to e_z, or

$$e_x = 0.07\ hu_* \tag{37}$$

The value of D_x has considerably more significance, and it has been analytically treated by Elder (42) following Taylor's approach. Elder determined the rate of transfer of material across a section(moving at the mean velocity of the fluid) due to differential advection. He used the logarithmic velocity profile with the origin at the water surface to find the advective portion of D_x to be

$$D_{xa} = \frac{0.404}{§^3} hu_* \tag{38}$$

in which D_{xa} = portion of D_x due to differential advection

§ = von Karman's constant

For the standard value of von Karman's constant of 0.4, $D_{xa} = 6.31\ hu_*$. The relationship is often approximated by

$$D_x = 6hu_* \tag{39}$$

This is due to the fact that $D_x = D_{xa} + e_x$, and e_x is much smaller than D_{xa}. In addition, Sayre and Chang (10) investigated the influence of a different velocity profile on the integrated result. For a parabolic velocity distribution, they obtained

$$D_{xa} = \frac{0.457}{\S^3} hu_* \qquad (40)$$

As they note, this is in surprising agreement with Equation (38) considering the usual assumption of extreme sensitivity to even small changes in the vertical profile. Ellison (55) and Bowden (56) used different assumptions and obtained values up to $25hu_*$. However, the most commonly used value is $6hu_*$.

Several experimenters have reported values which generally confirm this range of values. They all tend to be a bit higher, possibly because the existence of sidewalls in laboratory flumes may make the flow not truly two-dimensional, or for other reasons. Elder (47) himself reported values of $6.3hu_*$ experimentally. Fischer (20) reported on 197 experiments, with an average value of $13hu_*$, the range being from $10.4 - 15.7\ hu_*$. Thackston and Krenkel (57) reported similar results and Sayre and Chang (10) reported $5.3hu_*$ for three experiments.

In summary, the value of D_x is usually taken as $6hu_*$. In addition, as D_x includes no lateral averaging it provides a minimum value for any longitudinal mixing term in a two-or one-dimensional equation. If any lateral variation of velocity or concentration exists and is included in the coefficient definition, then the coefficient values must be larger than given by Equation (38).

The value of D_L, the longitudinal dispersion coefficient, is subject to a great deal more variability and much less certainty in selection. Table 3 shows typical values obtained experimentally. The variation illustrates the range of physical phenomena operative at different sites. In addition, however, it should be noted that in some instances the data reported here

or elsewhere may not have met the criteria for application of the one-dimensional equation. Data in the table are adopted from Fischer (8) and Liu (58).

TABLE 3. REPORTED VALUES FOR D_L

Reference	Channel	Depth, cm	D_L/hu_*
59	Chicago Ship Canal	807	20
60	Sacramento River	400	74
61	River Derwent	25	131
52	South Platte River	46	510
62	Yuma Mesa Canal	345	8.6
20	Trapezoidal Lab Channel	2.1-4.7	150-392
63	Green-Duwamish River	110	120-160
54	Missouri River	270	7500
64	Clinch River	58-210	210-800
64	Copper Creek, VA	40-85	220-500
64	Powell River, TN	85	200
65	Sinuous lab flume	2.3-7.0	5.8-35

It can be seen that the Missouri River value is far larger than any of the others. With the exception of this, most values reported here or elsewhere for D_L are less than $1000hu_*$. McQuivey and Keefer (66) report a number of other results, although they do not report the depth and hence the dimensionless coefficient value cannot be obtained. It is a useful set of data to review, however. All the data served to show the need for site-by-site reviews of the situation to enable prediction of D_L. Some simple predictors are reviewed in the next section.

4. Predictors for Longitudinal Dispersion Coefficient- Several simple means of selecting values for D_L have appeared in the literature and are presented here. It is essential to recall in reviewing any data appearing

in the literature that values obtained for D_L by use of the one-dimensional equation are only valid if the criteria for use of that equation have been met.

Fischer's analytical relationship (2) [Equation (20)] provides an excellent theoretical basis, but it requires a knowledge of the detailed velocity distribution in the section. Several workers have employed it in numerical schemes for routing material down long stretches of river. In fact, this use is usually referred to as Fischer's routing procedure.

Jain (67) has employed Fischer's Equation (20) with the lateral velocity variation suggested by Equation (21) (showing uh proportional to $h^{5/3}$) to arrive at a predictive equation for D_L for an idealized cross-section which is constructed to represent the real section. His equation is

$$D_L = \beta_J \frac{u^2 B^2}{D_y} \tag{41}$$

in which

u = mean velocity

B = channel width

β_J = coefficient, calculated, varying from about 10^{-4} to 10^{-2}

Means of determining β_J are given by Jain (67).

Liu (58) based his relationship on somewhat limited data. He had a screening procedure for elimination of some data which has drawn criticisms. His equation is

$$D_L = \beta_L \frac{u^2 B^2}{h u_*} \tag{42}$$

in which

$$\beta_L = 0.18 \left[\frac{u_*}{u}\right]^{1.5} \tag{43}$$

The expression is derived by best fit and fits the data on which it is based within a factor of 6. It should be noted that many researchers have been very happy to be able to fit data and predict the resultant coefficient within a factor of 4-6, giving an indication of the state of the art. Christensen (68) discussed Liu's paper and provided a theoretical basis for selection of a different expression for β_L which fits the data at least as well. His expression is

$$\beta_L = 0.41 \left(\frac{u_*}{u}\right)^2 \tag{44}$$

McQuivey and Keefer (66) have provided another equation based on fitting to field tracer data by use of Fischer's routing procedure to obtain the value of D_L giving the best fit to downstream concentration vs. time curves. They rely on information available for one-dimensional flow routing to derive the approximate relationship

$$D_L = 0.058 \frac{Q_o}{S_o B_o} \tag{45}$$

in which

Q_o = discharge at steady base flow

S_o = slope of energy gradient at steady base flow

B_o = width of channel surface at steady base flow

McQuivey and Keefer report that Equation (45) has a standard error of approximately 30 percent based on data over a wide range of flow conditions for 18 streams and 40 time-of-travel studies. This relationship has the advantage over Jain's that the value of D_y is not required, but this is not a major factor with all the other uncertainties.

Harleman (27) presents an expression based on Elder's and Taylor's work

for use in estuaries. Since it is based on this earlier work it therefore relates to vertical variation of velocities and therefore is more appropriately a descriptor of D_x, rather than D_L. However, it will be noted that in estuaries the time scale is frequently short enough that D_L is well approximated by D_x. The expression can be written as

$$D_x = 77nuR^{5/6} \tag{46}$$

in which

n = Manning's roughness coefficient

u = instantaneous velocity, ft/sec

R = hydraulic radius, ft

all in foot-second units

Fischer (69), in a discussion of Reference 66, proposed another equation, given as

$$D_L = \frac{0.011\, u^2 b^2}{hu_*} \tag{47}$$

A final statement seems in order. All of the equations presented herein are intended only as guides. None has been shown innately superior to any other. None can be expected to completely replace judgment and knowledge of the site. Each one may provide a useful first cut assessment where a preliminary estimate is required prior to any field studies.

FACTORS INFLUENCING COEFFICIENT VALUES

In the succeeding sections, a number of the most common factors affecting values for the coefficients will be discussed as knowledge exists for coefficients in each of the directions. It should be recognized that all of these modifications to basic values of the coefficients represent the lumping of advective terms into the coefficients, as discussed in Section II. It must be

noted then that some points will be reached where no amount of modification of the coefficients will enable accurate prediction of correct mixing behavior, especially over a long reach of the river where conditions may change considerably from point to point.

1. **Density Differences Between Effluent and Receiving Water** - Many materials are clearly strongly influenced by their density relative to the surrounding water to which they are discharged. Lighter materials tend to rise to the surface due to buoyant forces, while heavier ones tend to plunge. The momentum changes created by these density differences may in fact give the effluent a trajectory different from the ambient fluid and therefore change the total turbulence levels at the plume boundary to give behavior more like that of a jet of fluid into a receiving ambient fluid. For this reason, some people classify effects due to these density differences as part of the so-called mixing phase, in which discharge characteristics and momentum may dominate ambient mixing processes.

Edinger and Polk (70) note that heated water discharges in the field, when fitted to a diffusion model, yield values for the lateral coefficient larger than expected and values for the vertical coefficient smaller than expected. This is due to the increased lateral spreading due to the lighter heated water trying to ride up over the surface, while vertical mixing is restricted by the density gradient. Sonnichsen (71) reported similar findings.

The most comprehensive work in this area has been presented by Prych (45) and its use summarized by Brooks (72). Prych performed an extensive series of laboratory experiments in which effluents were discharged in the center of a channel in the same direction at the same velocity as the ambient flow. A number of runs (reported in Table 2) were made to establish the ambient level of turbulence in that particular laboratory flume. Then a series of runs were

made where the effluent was either heavier or lighter than the receiving water. His findings show that density differences enhance lateral mixing.

Prych deals with the variance of the lateral distribution of depth-averaged concentrations, σ^2, as a measure of the spread of material. His findings can be briefly summarized as below.

a. When $\Delta\rho$ (the density difference between effluent and ambient fluids) is not zero, $\sigma^2(x)$ is nonlinear up to some point and grows at a more rapid rate than where $\Delta\rho = 0$. This is shown in Figure 2, where it can also be seen that at large x, the curve becomes linear and parallel to the curve for no density difference.

b. Data indicates that the more rapid growth of $\sigma^2(x)$ is caused by density-induced secondary flows.

c. The dimensionless excess variance, $\Delta V = \Delta\sigma^2/h^2$, at large x shown on Figure 2, represents the added variance or spreading due to the density difference. ΔV is defined in Figures 3 and 4 and can be seen to be a function of only M_b (or M_d) and B'. In these figures

$$X = \frac{x}{\bar{u}} \frac{\alpha u_*}{h} \tag{48}$$

$$B' = b/h = \text{dimensionless source width} \tag{49}$$

$$M_b = \frac{\Delta\rho}{\rho_a} gb/(\alpha u_*)^2 \tag{50}$$

$$M_d = \frac{\Delta\rho}{\rho_a} gh/(\alpha u_*)^2 \tag{51}$$

in which

b = source width

ρ_a = ambient fluid density

α = D_y/hu_*

g = acceleration due to gravity

h = depth

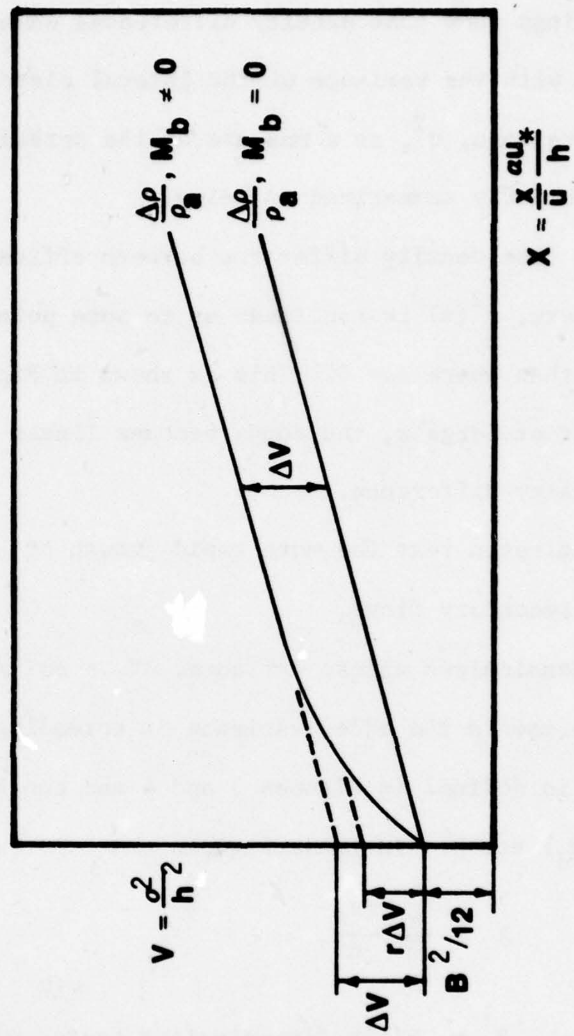


Figure 2. Increased Variance Due to Buoyancy
[After Prych (45)]

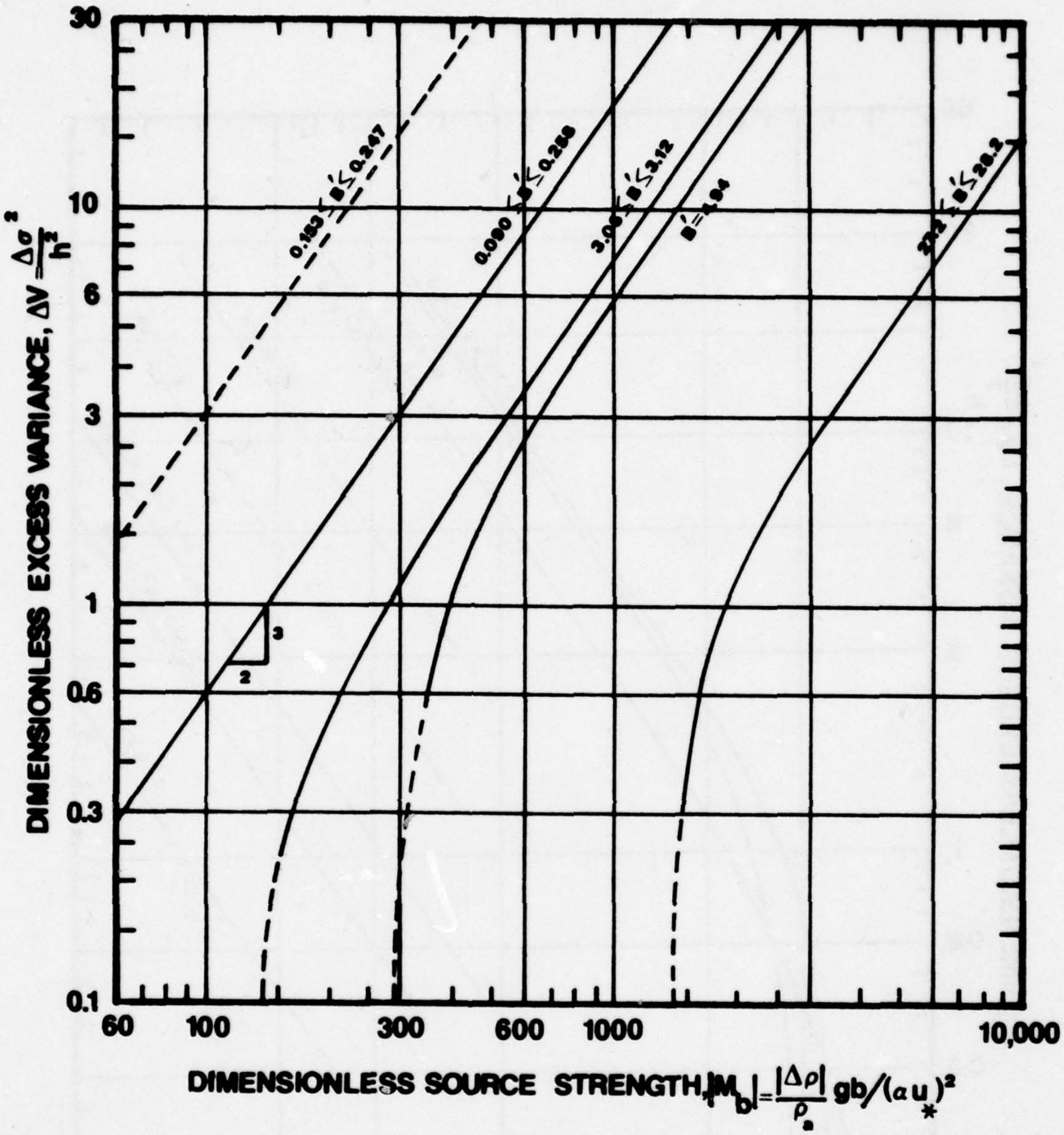


Figure 3. Dimensionless Excess Variance As a Function of M_b [After Prych (45)]

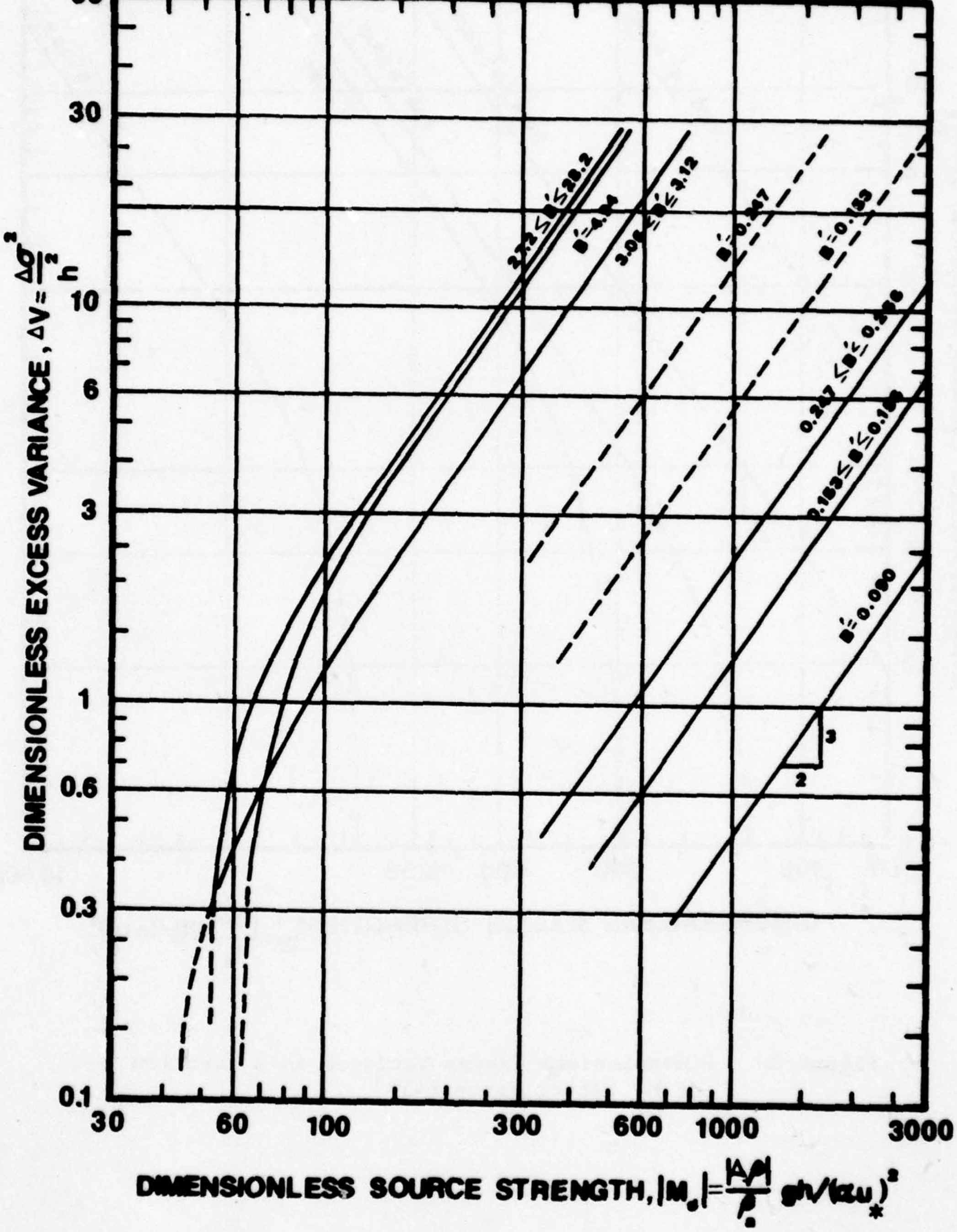


Figure 4. Dimensionless Excess Variance as a Function of M_d [After Prych (45)]

d. Evidently fluids which are more dense do not exhibit as much increase in spreading as lighter fluids for typical discharge cases. For B' much less than 1 (source width much less than the depth) and M_b constant, ΔV for fluids lighter than ambient is about 5 times the value for effluents heavier than the ambient. However, for B' much greater than 1 (source width much greater than depth), ΔV is the same for light and heavy fluids.

e. The variance can be predicted as a function of x by using the expression

$$V(X,B,M_b) = 2X + \frac{B'^2}{12} + r\,\Delta V \tag{52}$$

in which $V = \sigma^2/h^2$

r = function defined in Reference 45, giving the slope of the variance versus x curve in Figure 2

f. The excess variance is a one-time added spreading of the tracer fluid which occurs within a distance of about

$$\frac{x}{h} < \frac{1.5u}{\alpha u_*} \tag{53}$$

It is possible to convert Equation (52) to a form similar to a coefficient expression using the relationship from Reference 46,

$$D_y = \frac{1}{2} u \frac{d\sigma^2}{dx} \tag{54}$$

Using Equations (52) and (48), one can then write

$$D_y = (\alpha u_* h) + \frac{1}{2} uh^2 \Delta V \frac{dr}{dx} \tag{55}$$

The value of dr/dx reaches zero at or before the point defined by Equation (53). Earlier values can be obtained from Prych's data plots. Note that the first term on the right hand side of Equation (55) is the standard value of D_y, and the second term is an increment due to $\Delta\rho$ which ultimately becomes zero. Note that this D_y value in Equation (55) varies with x, although Prych's data indicates that dr/dx is reasonably constant over a broad range, generally up to about two-thirds of the distance given by Equation (53).

2. Stratification in Receiving Water - Less work has been done defining the effect of existing ambient stratification on diffusion processes. A few works are worthy of note, however.

(a) Sumer - Transverse Mixing - Sumer and Fischer (73) and Sumer (74) have reported on experiments measuring transverse mixing in oscillatory flows, both in uniform and non-uniform channels. In the uniform channel, the value of $\alpha = \frac{D_y}{uh_*}$ generally decreased as the Richardson number, R_i, approached 1, where

$$R_i = \frac{(\frac{\Delta\rho}{\rho})gh}{u^2} \qquad (56)$$

in which $\Delta\rho$ = density difference between upper and lower layers. In other words, D_y decreased as the stratification increased. The work gave values of α as $0.058 < \alpha < 0.273$ for the average over the depth.

In the non-uniform channel runs, α increased about 50 percent above the standard values for homogeneous ($\Delta\rho = 0$) runs, yielding

$$0.024 < \alpha < 0.50$$

For stratified runs, the range was

$$0.21 < \alpha < 1.87$$

Instantaneous salinity measurements show a lateral gradient of salinity toward the deep side, i.e., heavier water is always at the shallower side. It is surmised that these gradients may be established by vertical mixing induced by channel irregularities. The gradients in turn induce transverse circulation and hence larger values of D_y. Sumer (74) reports on an analysis similar to one outlined by Prych (45) in which the transverse velocity in a single cell is predicted and the value of D_y including these transverse velocities is calculated as $D_y = 0.953$, which is within the range of experimental values. This analysis lends credence to the belief that induced transverse velocities create the larger transverse mixing.

The results of Sumer's work show that the transverse mixing in a uniform channel is decreased by the existence of a stable density gradient in about the same proportion as the vertical mixing is reduced. In addition, a relationship between the coeffieient and a Richardson number can be discerned. However, few natural channels are uniform, and Sumer's results show that D_y is increased if the channel is irregular. Sumer and Fischer (73) note that it seems likely that the same holds for D_z, but they did not investigate this aspect. "Most numerical models of stratified estuaries hypothesize a relationship between mixing coefficients and some form of Richardson number. The results of this study suggest that in natural channels no such relationship may exist, or if it does, it may be in the opposite direction from what has usually been assumed." (73, page 599)

(b) Thatcher - Longitudinal Mixing in Salinity Intrusion Regions - Thatcher and Harleman (75, 76) have reported on application of one-dimensional models in salinity intrusion regions in estuaries. They recognize the role of the longitudinal density variations in the momentum equation and in the dispersion term. They suggest the following relationship for the longitudinal dispersion term in that case.

$$D_L(x,t) = K \frac{\partial s_*}{\partial x_*} + E_T \tag{57}$$

in which

K = coefficient defined in Equation (58)

$S_* = S/S_o$

S = Salinity

S_o = reference salinity

$X_* = X/L_o$

L_o = total length of estuary

E_T = Taylor's expression for the longitudinal coefficient

Taylor's value is obtained by

$$E_T = 100nR^{5/6} U_{max} \tag{58}$$

in which U_{max} = maximum tidal velocity.

This is a modification of Equation (46) to enable using a constant value over the tidal cycle. The coefficient K was found empirically to fit the relationship

$$\frac{K}{u_o L} = 0.002 E_D^{-0.25} \tag{59}$$

in which u_o = maximum cross-section velocity at mouth of estuary

$$E_D = \frac{P_T F_D^2}{Q_f T} \tag{60}$$

$$F_D^2 = \frac{u_o}{gh \quad \Delta\rho/\rho} \tag{61}$$

in which P_t = tidal prism (volume swept out by one tidal period)

T = tidal period

Q_f = freshwater inflow

It can be seen from these relationships that higher stratification implies a higher D_L value. This occurs due to the longitudinal salinity (density) gradient in the estuary.

(c) Fischer's Analysis - Fischer (24, 25) has presented the most comprehensive analysis of the factors contributing to estuarine circulation and mixing. This work will be reviewed more fully in the next section. It is clear that density differences do cause a part of the circulation in a real estuary, but Fischer (24) notes that much remains to be done in understanding real, irregular channels as three-dimensional problems where a number of factors - buoyancy, tidal momentum input, currents due to irregular channel geometry, and the like - all interact. As he notes, even in cases where vertical mixing appears complete there may be significant density-driven circulation.

3. Flow Unsteadiness - As might be expected, this is a complex topic about which much has been written and speculated but where much remains to be done. A number of earlier comments have been made about various unsteady flows for other reasons, e.g., non-tidal advective models, Sumer's (74) work on transverse mixing, and Thatcher and Harleman's (75) work on salinity intrusion. Most work on unsteady flows has been in estuaries, but the same phenomena exist in unsteady river flows. In fact, especially where rivers are controlled by dams, there can be flow reversal. Brocard and Harleman (77) and Daily and Harleman (78) have developed a generally applicable one-dimensional model, and the former workers have applied it to Conowingo Reservoir, a controlled river reach.

In keeping with the tenor of this report and its goal to provide useable results only a brief review of current thought will be presented, along with some brief guidance to enable coefficient selection in unsteady cases.

(a) Fischer Review - Fischer (24) has prepared an excellent discussion of the physical phenomena involved and tried to classify the mechanisms which circulate material. The reader interested in a detailed literature review is strongly urged to read this article. It provides a very good list of references up to the time of the review (1976). Fischer also draws heavily on an analysis of circulation he performed (25). An estuary in steady state (from cycle to cycle) has the net seaward transport by the mean outflow balanced by three terms representing landward transport by a variety of mechanisms. The three terms represent (a) trapping, (b) residual currents (gravitational, pumping, and wind), and (c) shear effect plus unsteady wind effects.

"Trapping" represents retention and delayed release of material by embayments or tidal shoals or other local geometry features. This trapping has the effect of spreading the material out along the estuary axis, resulting in a larger apparent value of D_L.

The most significant form of residual current is that due to gravitational circulation, caused by the density distribution. Inertial and frictional effects, the earth's rotation, and wind also contribute to the residual circulation. Most studies to date have dealt with the vertical circulation. In addition, many lab studies have employed rectangular flumes. Fischer (24) reviews findings on the vertical circulation, but he then states (25) that a non-rectangular section would contain a transverse circulation. This circulation was computed to be landward in the deeper parts of the cross section and seaward in the shallower parts. Fischer applied this concept to data taken on the Mersey estuary and found that the transverse gravitational circulation should contribute about 90 percent of the magnitude of the dispersion coefficient there. In that case vertical mixing was achieved 18 times as rapidly as transverse mixing.

All of this implies that there is still a shortage of readily applicable information on this obviously important mechanism. Fischer notes that work should move "...towards a three-dimensional understanding of gravitational circulation, and towards an understanding of the interplay between the buoyancy input from the river and the momentum input from the tide in generating the distribution of currents in real estuaries." (24, page 121)

"Pumping" is that portion of the residual circulations due to tidal waves interacting with the channel boundaries. Fischer (24) gives some examples.

The wind may enhance local mixing due to surface wave generation, but its primary impact may be due to its generation of currents in the water body. These currents are strongest nearest the surface, generally being 3-5 percent of the steady wind speed (79). These may enhance (or retard) already existing advective velocities in the longitudinal direction or create additional transverse velocities. The author has observed a site on the Mississippi River near a large thermal discharge where the wind made significant differences in thermal plume behavior. The plume vertical extent was on the order of 10 feet, so that it was subjected to the greatest induced surface currents. Two consecutive days with similar plant discharges and almost identical river flows yielded widely different areas influenced by the thermal plume. A very steady wind existed from the north on the second day with a magnitude of 16 to 18 miles/hour. This would create surface currents comparable to the normal stream velocities of about 1 ft/sec at the low flows being studied.

Fischer (80) provides a numerical example of the relative importance of the various mechanisms in the Northern San Francisco Bay, which consists of a series of large bays joined by narrower channels. A one-dimensional analysis is probably not appropriate for this case, but Fischer and Dudley make reasonable assumptions to estimate effects. They observe that vertical gravitational circulation is unlikely to account for the observed length of salinity intrusion, whereas the combined effects of trapping, pumping, and wind are entirely capable of doing so. Fischer (24) notes that numerical models are adept at handling trapping and pumping, but less capable of handling gravitational circulation. This may explain the reasonable results obtained from applying numerical models to San Francisco Bay, with lesser success at other sites. Fischer notes that "...it is useful to begin a study of an estuary by evaluating which mechanisms are important." (24, page 127)

(b) Estimate of D_x in Estuaries - An expression is shown in Equation (46) and later modified in Equation (58) for D_x in tidal estuaries. This D_x is the same as the E_T showing up in Equation (57). As Fischer (24) notes this E_t is misnamed the Taylor result because Equation (46) was originally obtained rather arbitrarily by modifying Taylor's result for a circular pipe. The step from Equation (46) to (58) is made based on work by Holley and Harleman (81). They conducted experiments which showed that a single constant value for the dispersion coefficient could be assumed throughout the tidal cycle if the time average value of the absolute value of the tidal velocity is used. If the tidal velocity varies sinusoidally in time, then this time average value is $2/\pi$ times U_{max}. The resulting equation is then increased by a factor of 2 to account for increases in longitudinal dispersion due to bends and channel irregularities. Hence, Equation (58) is the final recommended form.

(c) Holley, et al Dispersion Due to Shear - This is really the third category of landward transport mentioned by Fischer (24) and is the closest to the type of motion previously discussed in Section II of this report. Holley, et al (82) and Fischer (83) have studied dispersion in constant density portions of oscillating flows. They have both noted that the time scales of vertical and horizontal mixing relative to the time scale of oscillatory motion controls the behavior of a dispersing material. "For any net dispersion to occur, the period must be great enough for some cross-sectional mixing to take place. Then, for example, a particle carried one direction by a high-velocity streamline may migrate by diffusion and return by a lower velocity stream line, and longitudinal dispersion will take place." (82, page 1697)

Consider a cross-sectional mixing time, T_c which will be different for vertical and transverse directions. Further, define

$$T' = \frac{T}{T_c} \tag{62}$$

in which T = period of oscillation. If T approaches infinity, this represents a steady-state case. From a practical standpoint, if T' is greater than one, the coefficient of interest will be able to attain its steady-state value. Bowden (84) found that a sinusoidal velocity which varied spatially both vertically and transversely gave a value of one-half that of a steady flow with its velocity equal to the peak tidal flow. Okubo (85) noted that the value was dependent upon T', with Bowden's result valid for T' much greater than one.

On the other hand, Holley, et al (82) investigated the variation for smaller T' where only a vertical velocity gradient existed. They presented a curve and an approximate equation for the variation, ranging from a zero value of the coefficient at T' = 0 to the maximum, steady-state value at T' approaching 10. That equation giving the average value of the dispersion coefficient over a tidal cycle is written as

$$\frac{D_x}{D_{x_\infty}} = \frac{240T'^2}{\pi^4} \sum_{n-1}^{\infty} \frac{1}{(2n-1)^2 \left[\frac{\pi}{2}(2n-1)^2 T'\right]^2 + 1} \tag{63}$$

in which D_{x_∞} = dispersion coefficient for steady flow.

This equation was derived with numerous simplifying assumptions, but it gives a good general view of the variation with T'. They introduce separate time scales for vertical and transverse mixing, with

$$T_t' = \frac{T}{T_{c\ \mathrm{trans}}} = \frac{T}{\frac{b^2}{e_y}} \tag{64}$$

$$T_v' = \frac{T}{T_{c\ \mathrm{vert}}} = \frac{T}{\frac{h^2}{e_z}} \tag{65}$$

in which b=channel half-width = B/2. Holley, et al (82) do some order of magnitude review and observe that for most estuaries, T_v' is much greater than 1.0, while T_t' is less than 0.1.

This means that the full degree of longitudinal dispersion due to vertical velocity gradients is always achieved, but only a fraction of the contribution due to transverse gradients is realized. They propose a preliminary equation for the ratio $\frac{E_t}{E_v}$, where $E_t = D_v$ = dispersion coefficient based on transverse variations, and $E_v = D_x$ = dispersion coefficient based on vertical variations. Their equation, valid only for $T_v' > 1$ and $T_t' < 0.1$, is

$$\frac{E_t}{E_v} = 0.011 \left(\frac{U_T T}{b}\right)^2 \left[\frac{\overline{u''^2}}{(\frac{2}{\pi} U_t)^2}\right] \tag{66}$$

in which

U_T = maximum tidal velocity

u'' = deviation between cross-sectional mean velocity and velocity at any given point in the section.

Obviously, evaluation of this ratio requires a knowledge of the spatial distribution of velocities so that u" can be determined throughout the section. As a guide, Holley, et al (82) used values of 0.01 and 0.04 for the bracketed expression on the right side of Equation (66) and note that its value would be about 0.02 for a logarithmic velocity distribution. This equation is based on Fischer's (20) simple result comparable to Equation (20), or

$$\frac{D_L}{Ru_*} = 0.30 \frac{\overline{u''^2}}{u_*^2} \left(\frac{L}{R}\right)^2 \tag{67}$$

in which R = hydraulic radius

L = distance from thread of maximum velocity to most distant bank

This equation has not been verified for geometries typical of estuaries and represents only an attempt to try to understand the relationships between parameters. Therefore, no real exactness should be associated with its use. It does provide a reasonable first step toward evaluation of the relative impact of velocity variations in the two directions. They recommend the following procedure for defining D_L.

(1) Calculate T_t' and T_v' .

(2) If $T_t' < 0.1$ and $T_v' > 1$, use Equation 3.35 to calculate E_t/E_v.

(3) If $E_t/E_v < 1$, vertical variations of velocity dominate the dispersion, and $D_L = D_x = 6\ hu_*$. [Equation (39)].

(4) If $E_t/E_v > 1$, more detailed information is needed about the transverse variation of velocity to enable evaluation, for this variation dominates the process and may yield a coefficient whose value approaches 10 D_x .

(5) They note that if the discharge is a continuous one, then the factor of 10 in the coefficient may not be significant and use of $D_L = D_x = 6hu_*$ may be satisfactory. However, this is not true for unsteady discharges of material such as occurs in a spill.

It is worth noting that if the rate of transverse mixing is enhanced above standard levels by bends, groins, islands or sandbars in the flow, or the like, this further increases the possibility that the transverse contribution will dominate. In general, then, it seems likely that for wide estuaries the value of D_L can be approximated by $D_x = 6hu_*$, while for narrow estuaries or those in which the rate of transverse mixing is high the coefficient must be estimated based on a measured or assumed transverse velocity variation.

Harleman (27) mentions the example of the upper Delaware Estuary. There, it is estimated that T_v' is about 15, while T_t' is about 1/200. It could be concluded for this case that the vertical variation dominates and D_L can be taken as $6hu_*$.

The preceding discussions cover many elements and are often based on preliminary sorts of equations. For this reason, the predictive equatio.s of, e.g., Holley, et al (82) are given here only for preliminary analyses. The major significance of what has been said lies in the importance of the mixing time scale. Calculation of T_v' and T_t' enables a first estimate of the relative importance of the mixing mechanisms. Further evaluation of the coefficient values ranges from simple (if vertical variations control and $D_L = 6hu_*$) to complex (if E_t controls). This situation is consistent with the previous discussions indicating the large degree of uncertainty associated with coefficient selection in estuaries. Recall that there are many factors in addition to the shear behavior discussed here. Holley, et al (82) note that their analysis is probably most nearly applicable to estuaries which have a well-defined and reasonably straight channel, such as those found along the east coast of the United States. It probably does not apply to multi-channeled or island-laden estuaries similar to portions of the Columbia River. For estuaries where other major mechanisms - overbanks, shoals, islands, bends, or other gravitational circulation - are not apparently important, the information presented here can provide some guidance to coefficient selection. The final decision will have to rely also on judgment.

d. Ward's (86) Work on Transverse Mixing in Oscillating Flows - Ward (86-88) performed laboratory tests and reanalyzed field data on transverse mixing in oscillating flows, providing additional information on the influence of bends and channel geometry on this process. In his laboratory work, he varied the flow depth, h, and the radius of curvature of the bends, R_c. He additionally used the parameter $L_* = B/2$, where B = channel width. He found he could categorize the time average value of the transverse mixing coefficient in two ways, using either the average value of the shear velocity or the instantaneous value. This yielded

$$\frac{D_y}{h\bar{u}_*} = fn\left(\frac{L_*}{R_c}, \frac{h}{R_c}\right) \tag{68}$$

$$\frac{D_y}{hu_{*o}} = fn\left(\frac{h}{R_c}\right) \tag{69}$$

in which $\bar{u}_*$ = time average value of u_*

u_{*o} = instantaneous maximum flood tide value

These relationships are illustrated in Figures 5 and 6. Figure 5 shows the relationship in Equation (68), with values for the dimensionless coefficient, or α from Equation (32), ranging up to about 1.7. When the representation of Equation (69) is used, Figure 6 shows values of α all less than 1.0 for the ranges tested. Notice that these values are in the ranges of values reported by Sumer (74). In his study, secondary currents were generated by channel non-uniformities and flow stratification, while in Ward's work they occurred due to bends. Ward also reported three estuarine cases for which he found data where the α value obtained by dividing by $\bar{u}_*$ as in Equation (68) ranged from 0.42 - 1.03.

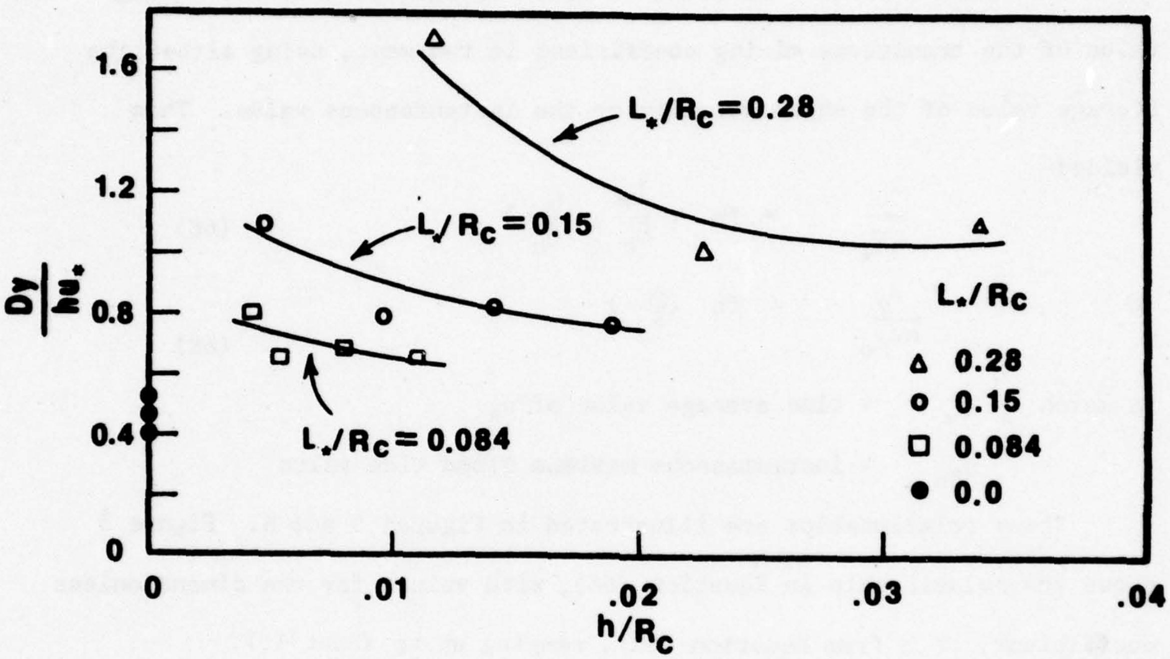


Figure 5. Transverse Mixing Coefficient in Oscillating Flows Using Average Shear Velocity [After Ward (86)]

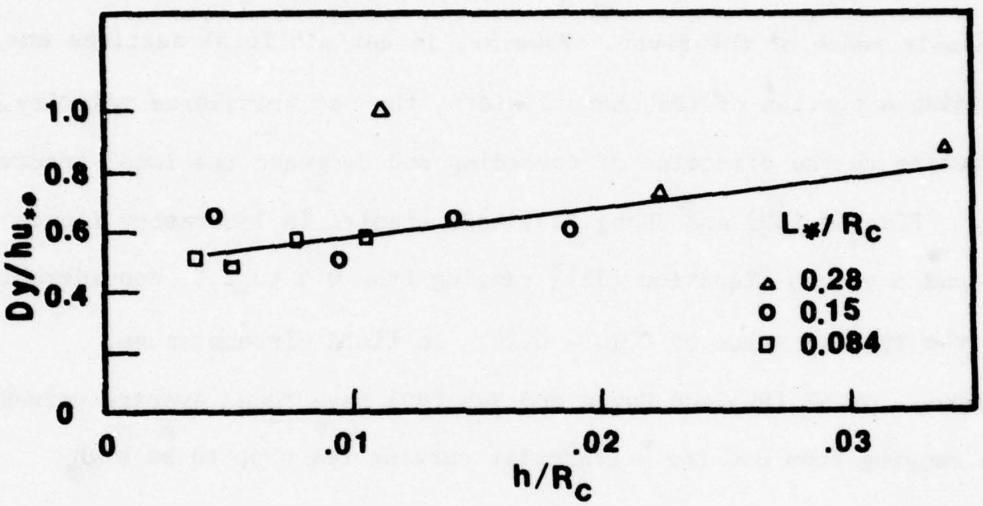


Figure 6. Transverse Mixing Coefficient in Oscillating Flows Using Peak Shear Velocity [After Ward (86)]

4. Bends and Other Geometry Problems - The primary effect of any geometry feature lies in its tendency to (a) induce currents in the flow and (b) to limit available dilution water by the existence of a limiting boundary. A number of these effects have already been discussed in earlier sections. Some other works will be reviewed here.

a. Transverse Mixing in Bends - In bends, the secondary current, helical in nature, has the effect of enhancing transverse mixing over a reasonable reach of the river. However, in certain local sections encompassing a portion of the channel width, the net transverse velocity may be opposite to the direction of spreading and decrease the local transverse mixing. Fischer (89) and Chang (13) made studies in laboratory flumes and found α values [Equation (32)] ranging from 0.5 to 2.5, considerably above the typical value of 0.10 - 0.20. In field circumstances, Yotsukura, et al (54) and Sayre and Yeh (40) have found average values for α ranging from 0.6 for a gradually curving reach up to as high as about 10 for a very sharp bend. However, it appears that other elements, specifically groins along the shoreline (on the Missouri River) may have contributed to this very high value by generating added transverse currents.

Fischer (89) employed Rozovskii's (90) radial velocity distribution to derive the expression

$$\frac{(\Delta D_y)}{hu_*} = \left(\frac{\bar{u}}{u_*}\right)^2 \left(\frac{h}{R_c}\right)^2 \frac{I}{\S^3} \tag{70}$$

in which $\S$ = von Karman's constant

ΔD_y = increment due to helical motion

R_c = radius of channel curvature

I = function given in Reference 89, varying from 0.02 to 0.2

This result was for an infinitely wide channel, with no boundary influences. Sayre and Yeh (40) have found improved correlation with data by including the factor B/h, the width-to-depth ratio. Yotsukura and Sayre (38) plot field and lab data and show that in both cases α is proportional to

$$\left(\frac{B}{h}\right)^2 \left(\frac{\bar{u}}{u_*}\right)^2 \left(\frac{h}{R_c}\right)^2$$

Even this does not bring laboratory and field data together, implying that more work is needed. However, it does provide a useful guide to the effect of flow or geometry changes.

It is interesting to review Ward's data in Figures 5 and 6. Again, the same trend with h/R_c is evident in his work. Physically, one can realize that R_c approaching infinity implies a straight channel, and α values should decrease with larger R_c.

Krishnappan and Lau (19) have carried out a laboratory study where the bottom was allowed to deform in the way a natural channel would, i.e., deeper portion toward outer part of the bend, etc. The earlier studies had rigid beds of generally uniform depth. They used the generalized change of moments approach for data analysis proposed by Holley, et al (18), to separate out the spreading due to the net transverse velocity. The remaining coefficient represents spreading due to (1) turbulent diffusion and (2) differential convection due to the variation of the transverse velocity over the depth. The resulting α values varied between 0.213 and 0.416, larger than the usual 0.10 - 0.20 for a straight channel, but smaller than the values reported by Chang (13) and Fischer (89), which ranged up to 2.5. Note that these other two investigators used rectangular channels with flat bottoms, while Krishnappan and Lau used channels with large transverse variations in depth, as well as cross-section variations when moving downstream. It is clear that this difference in channels is the major factor causing differences in coefficients. It still leaves, however, many questions with respect to predicting the coefficients for any given site.

Holley, et al (18) review also the effect of bends. It is noted that as the flow proceeds through a series of bends, a lateral current exists due to the movement of the bulk of the flow from one side to the other. The deeper portion of the river section (and hence the major portion of the flow and the higher velocities, occur toward the outer part of a bend. Therefore, dependent upon where the release point is, there may be a tendency for the transverse currents to enhance (add to) mixing due to standard processes or to decrease it. In fact, Holley, et al (18) note that if this transverse velocity is not considered, it is possible to obtain negative values for diffusion coefficients by standard means of fitting data. Chang (13) in fact found this in his work.

Chang (13) summarizes some of his key findings as follows:

> 1. The lateral mixing coefficient in a meandering channel is closely related to the development and decay of the helical motion. It is periodic in the longitudinal direction. In general, maximum values occur near the downstream portion of bends, and minimum values occur in the upstream portion of bends. The mixing coefficient also depends on the lateral position of the plume and hence on the source position.
>
> 2. The lateral mixing coefficient can be approximately represented as the sum of a variable lateral dispersion coefficient and a turbulent diffusion coefficient.
>
> 3. The lateral dispersion coefficient, which relates the lateral convective flux across stream tube boundaries to the lateral concentration gradient, is negative at the beginning of the bend, where the helical motion reverses direction. When the lateral dispersion coefficient is negative the dispersant is convected by helical motion from a region of lower depth-averaged concentration to a region of higher depth-averaged concentration.
>
> 4. The normalized lateral dispersion coefficient D_y/hu_* was found to decrease with increase of roughness at the bed.
>
> 5. In a wide channel, the lateral dispersion coefficient should increase with increasing depth to radius-of-curvature ratio, as does the intensity of the helical motion. However, when the width-depth ratio is small the helical motion and hence the rate of lateral dispersion is evidently attenuated by the influence of the side walls. Therefore the lateral dispersion coefficient actually decreases with increasing depth to radius-of-curvature ratio. (13, pages 94-95)

In summary, processes in bends are very complex and provide a real problem in selection of proper coefficients. It is best to think of two separate kinds of problems: (1) a discharge which proceeds through a number of bends over a reasonable length of the river to the point where a prediction is needed, and (2) a discharge from a particular point in or near a bend where a predicted concentration is desired very near the discharge point. In the former case, elevated values of D_y/hu_* similar to those reported by Chang (13), Fischer (89), Ward (86), and Yotsukura, et al (54) are appropriate. In the latter case, judgment must be applied to understand the transverse velocities generated in the bend. The state of the art in this area is not too far along. The author feels that future work which incorporates transverse velocities in the model is more likely to adequately describe mixing processes in bends than using varied coefficients in a standard model. For the time being, however, it seems that Chang's work provides the best basis upon which to proceed.

The neglect of transverse velocities has been shown to be one factor resulting in larger transverse coefficients when data are fitted to a model. Holley, et al (18) note that transverse velocities on the order of one percent of the main stream velocity can give transverse spreading rates comparable to standard diffusion rates. The author has made comparisions of the magnitude of the neglected term, $v\ \partial c/\partial y$, as compared to the second derivative transverse diffusion term, using the solution for a point source discharging into an unbounded medium. It is clear that even values of v on the order of one to two percent of the mean longitudinal velocities yield a neglected term on the same order as the standard diffusion term over a large portion of the flow field for typical river-parameter values.

In addition, Sumer (73) has used a simplified analysis of the transverse velocity field and derived a value of α equal to 0.95 for a typical case. This clearly shows the impact of transverse velocities.

All of this does not necessarily mean it is necessary to go to a numerical model in two dimensions. It does mean, however, that use of any model requires consideration of potential sources of transverse velocities to enable assigning reasonable coefficient values.

b. Other Geometry Effects - Other peculiar geometry effects are as numerous as there are possible physical sites. Strange bank or bottom configurations, structures, attached water bodies such as embayments or pools are some examples. Sayre and Caro- Cordero (22) and Holley and Abraham (91) present findings relative to grion's which are control structures protruding from the bank. The high value of D_y/hu_* of about 10 reported by Sayre and Caro-Cordero in the Missouri is partly due to extensive groins in the area.

Holley (23) presents Figure 7 as a way of viewing transverse mixing rates with groins, also helping to illustrate behavior across bends as discussed earlier. In Figure 7, the component e_{u*} represents the contribution to diffusion by shearing action (the 0.1 - 0.2 hu_* portion), while e_h represents the contribution due to helical motion in a bend. Superimposed on this is increased turbulent mixing, represented by e_g, caused by the groins (or other structures protruding into the channel). It is to be expected that increased turbulence due to these structures will have a limited physical extent, thereby affecting only a portion of the width of a sufficiently wide river but the entire width of a narrower stream. In addition, it is evident that the behavior of the discharged material will vary according to (a) its location in the channel and (b) the portion of the channel it covers. This further emphasizes the need for site-by-site reviews, although it is clear that current information does not enable estimation of the extent of groin influence.

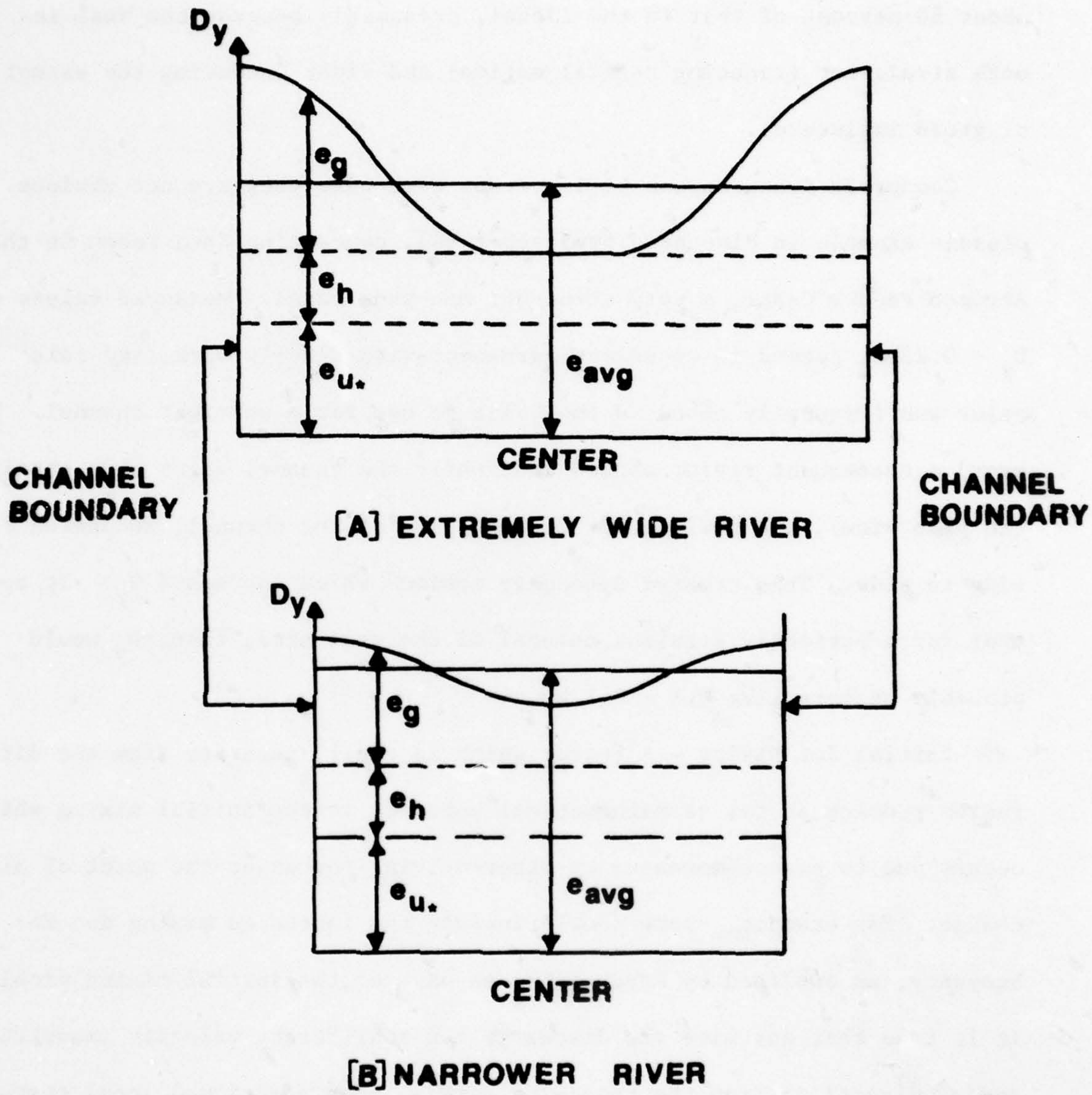


Figure 7. Contribution of Groins to Transverse Mixing
[After Holley (23)]

Holley and Abraham (91) report on the results of five field tests on two rivers in Holland. For the IJessel River, D_y/hu_* is about three times that for a straight rectangular channel. For the Waal River, D_y/hu_* is about 60 percent of that in the IJssel, presumably because the Waal is both straighter (reducing helical motion) and wider (reducing the extent of groin influence).

Geometric features can be important even when they are not obvious. A classic example is discussed by Fischer (8), concerning data taken in the Atrisco Feeder Canal, a very straight, man-made canal. Measured values of $D_y = 0.23hu_*$ seemed in excellent agreement with Elder's work, and this value was frequently cited as the value to use for a straight channel. However, a subsequent review showed that while the channel edges were straight (in plan view), the thalweg, or deepest part of the channel, meandered from side to side. This created secondary motions which increased D_y. It appears that for a perfectly straight channel of the same size, then, D_y would probably be more like 0.1 - 0.2 hu_*.

c. Initial Jet Mixing - A factor which is really separate from the diffusion problem as far as mathematical approach is the initial mixing which occurs due to excess momentum or other driving forces at the point of discharge. For example. some people include the increased mixing due to buoyancy, as outlined by Prych (45), as part of the initial mixing problem. It is true that any time the discharge has a different velocity (magnitude and/or direction) from the receiving stream, then additional local turbulence is generated by the shearing action between the two fluid streams. The key fact to note here is that the diffusion models discussed in this report are not applicable until this initial excess momentum is dissipated and the pollutant is subject only to ambient velocities. The same is also true in faster flowing receiving waters where the velocity of discharge is less than the ambient.

For cases where initial mixing is significant, a model linking this mixing with diffusion is needed. Some simple attempts have been made for steady state cases, but none for the unsteady discharges likely in a spill.

Sayre and Caro-Cordero (22) have developed a model based on empirical evidence for the dilution and spreading which occurs in the initial region at a site on the Missouri River. Eheart (26) has attempted to link a jet model to a diffusion model. These and other such linkages attempt to define the areal extent of the pollutant plume in the cross-section and the peak concentration at a point where initial mixing is assumed to have been dissipated. This gives a concentration and size to use as the source for the diffusion equation. Brooks (92) discusses use of an adjusted initial concentration after initial mixing, but uses it as a constant concentration over the newly-defined source, as others have done, rather than a more representative distribution. The interested reader is referred to sources such as those by Benedict, et al (93), Benedict, et al (94), and Jirka, et al (95).

d. Depth Variation in Receiving Waters - Some effects of depth variation have been previously mentioned, including the depth variation in bends which give rise to variation of transverse velocity across the stream. Krishnappan and Lau (19) note this effect. In addition, intuition leads one to the understanding that material entering shallow water near the channel bank will be diluted less rapidly due to the existence of limited quantities of water for dilution purposes. Holley, et al (18) report on some numerical experiments in which pollutant behavior in a rectangular channel is compared with that in a trapezoidal channel of comparable size and velocity. Considerably higher concentrations are noted in the shallow

regions of the trapezoidal channel. This sort of behavior is duplicated in many natural channels and in flows with overbank regions.

e. **Width-to-Depth Ratio in Channel** - The width-to-depth ratio has been cited in the discussions on bends and groins as having importance in the diffusion process. Earlier discussions on the scale of turbulence are important here also.

Okoye (46) has presented data on the effect of the width-to-depth ratio, shown in Figure 8. It is apparent that the aspect ratio, $\lambda = h/B$, has an effect. However, it appears that over a broad range the scatter in the data is sufficient to mask some of the variation and yield some uncertainty in selection of a coefficient. It does appear, however, that as λ approaches 1.0 (the channel gets relatively narrower) the value of α is reduced by the apparent limitation of the scale of mixing by the existence of the sidewalls. It also appears that somewhat higher values might be expected in relatively wide natural channels. For example, for B/h of 100, $\alpha = 0.25$ or more might be reasonable.

In a recent study, however, Lau and Krishnappan (96) have presented imposing evidence suggesting possible error in Okoye's suggested trend or at the very least showing uncertainty in the state of the art. They review Okoye's own data (note the scatter in Figure 8) and other data and note that it is hard to define a definite trend. They then present some of their own data and show what appears to be a very good correlation between B/h and D_y/u_*B. They do note that the friction factor, f, is obviously still a factor and variability of D_y with f remains to be better defined. They concluded that the dominant mechanism in transverse mixing is the secondary circulation driven by variations in transverse shear. This variation is governed by the width-to-depth ratio, as narrower channels find more of the flow region affected by sidewall shear and hence have larger secondary currents. This reasoning leads one to expect

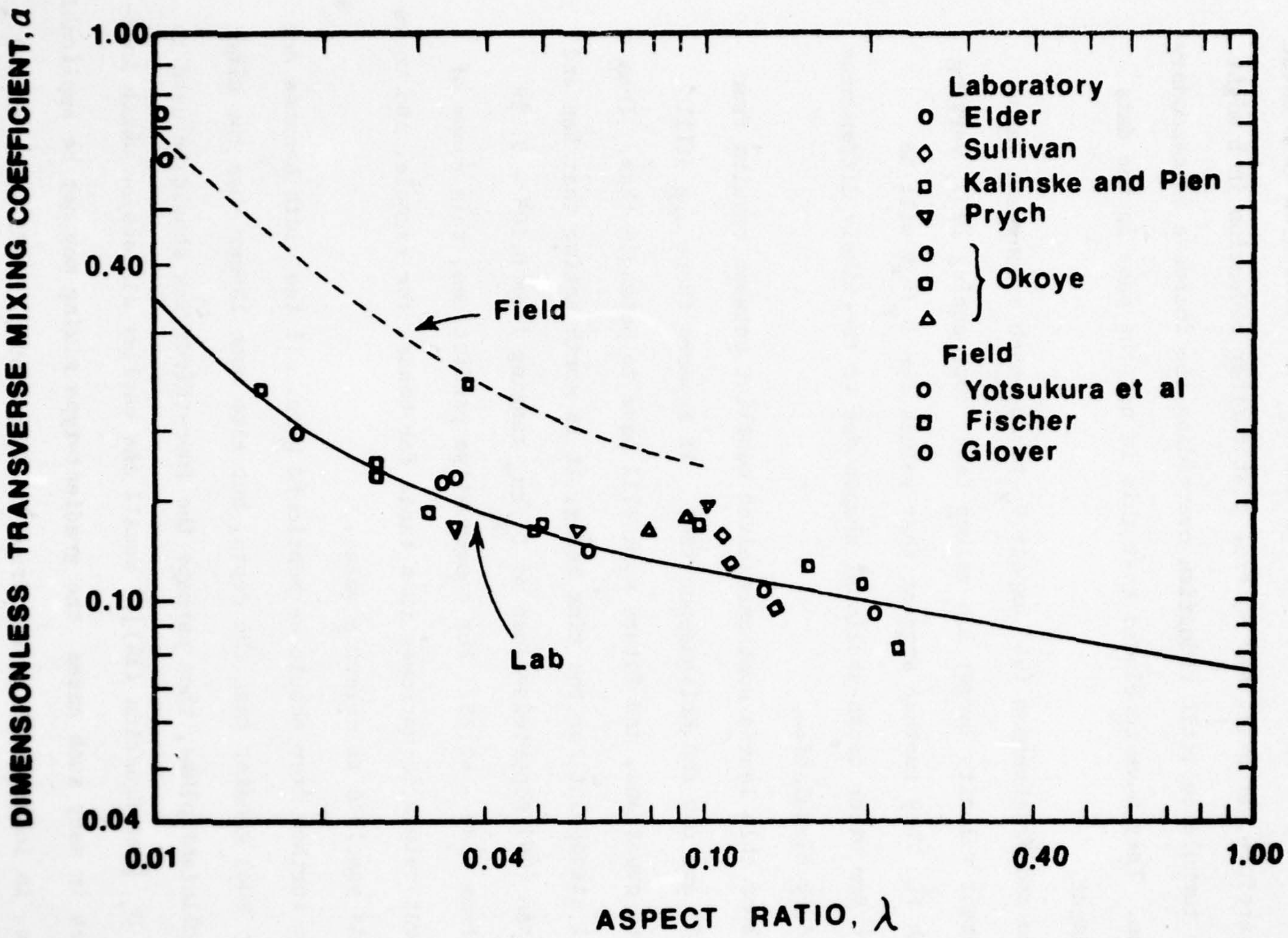


Figure 8. Influence of Width - To - Depth Ratio on D_y
[After Okoye (46)]

larger D_y values if the channel width is decreased. It should be noted that Lau and Krishnappan's results included no B/h value less than about 8.8. Therefore, it still may be true that further reduction in B might find the turbulence scale reduction overriding the increase in secondary influence. They have concluded that this is not the case in the data they present.

Lau and Krishnappan (96) expect D_y to approach a constant value for constant velocity larger B/h values (say, approaching 100), varying only with f. They further suggest that values for D_y/u_*B will be different for other cross-sectional shapes due to the likely differences in secondary circulation.

All of this leaves some unresolved conflict between results from Okoye (46) and Lau and Krishnappan (96). It appears there are still unanswered questions, and future work will have to untangle them. From a practical standpoint for the time being, it is worth noting that Lau and Krishnappan (96) reported values of D_y/hu_* ranging from 0.108 - 0.259 for B/h from 8.88 - 42.86. For conservative predictions, this range of coefficient values is narrower than those for bends, for example, and therefore it is possible to select a value.

One further item should be mentioned here. If the width becomes not only very much greater than the depth, but also much larger than the size of the pollutant plume, then perhaps the four-thirds law should be used to estimate D_y [see Equation (34)]. Recall the earlier discussion which indicates that in many such cases the gradient-type mixing may not be applicable. Therefore, in lakes or large estuaries or embayments, coefficients should probably be calculated by the four-thirds law.

APPLICABILITY OF 1-D MODEL

One of the errors most frequently made in analysis of water quality problems is the use of one-dimensional (1-D) models when in fact the process is not really 1-D. It has been established that there are some criteria which can be applied to determine the length downstream required to reach the point where the concentration is sufficiently uniform across the stream section to allow use of the 1-D, longitudinal dispersion equation [Equation (18)]. Fischer (20) and Ward (97) have presented criteria for estimating the longitudinal distance required to reach this point, with both methods giving comparable results. Fischer's equation yields

$$X_L = 0.4 \frac{uL^2}{D_y} \tag{71}$$

in which X_L = distance to point where Equation (18) applied

L = distance from streamline of maximum velocity to most distant stream bank

It can readily be seen that for wide streams a substantial distance (many miles) may be required to justify use of the 1-D equation. Therefore, even for problems where longitudinal behavior is of most interest, use of a two-dimensional equation such as Equation (15) may be best. In fact, Holly (98), in a discussion of the work by Liu (58), makes this point very well. He shows excellent fit to a set of data using the 2-D model, while the 1-D model gives a quite different trend.

Other investigators have dealt with the 1-D question also. Ruthven (99) has used the Fischer criterion in an assessment of applicability of the 1-D model for BOD. McQuivey and Keefer (100) note that about 150 miles may be required in a particular stretch of the lower Mississippi River for 1-D conditions to be met after a dye dump. It is not uncommon to see

estimates of X_L approaching this sort of large distance in larger rivers.

Fischer suggests Equation (71) as a criterion for estuaries also. In terms of time, the time required for a side discharge to mix completely across the cross-section (T_{mix}) is on the order of

$$T_{mix} = \frac{0.4\ B^2}{D_y} \tag{72}$$

Fischer (101) found that in a stretch of the Delaware Estuary about (1300 meters wide) about 10 days would be required for complete mixing. A one-dimensional model would therefore not be a good choice for a side discharge at that site. Fischer (24) notes that in many cases, material discharged into an estuary is flushed into the ocean before complete transverse mixing occurs and thus the 1-D equation has no value at all in those cases.

Ward's (97) results clearly show the effect of the location of the discharge point. As might be expected, material discharged near the center of flow reaches 1-D conditions most quickly, as spreading occurs in both lateral directions and must cover a shorter distance to reach the bank than where material is discharged from one bank. Both Ward (97) and Holley, et al (18) note the extreme importance of channel bends in increasing D_y and therefore decreasing X_L. Ward presents figures based on his numerical experiments, as do Holley, et al. The latter are shown here as Figures 9 and 10, which are illustrative of some important points.

It must first be noted that any practical definition of complete mixing must specify some allowable deviation across the channel, e.g., a maximum 2 percent, or 5 percent, variation across the channel. In Figure 9, the crossing distance, X_c, is defined as the point downstream where the concentration on the far bank first reaches 2 percent of the near bank concentration. (Discharge is from one bank into a rectangular channel.)

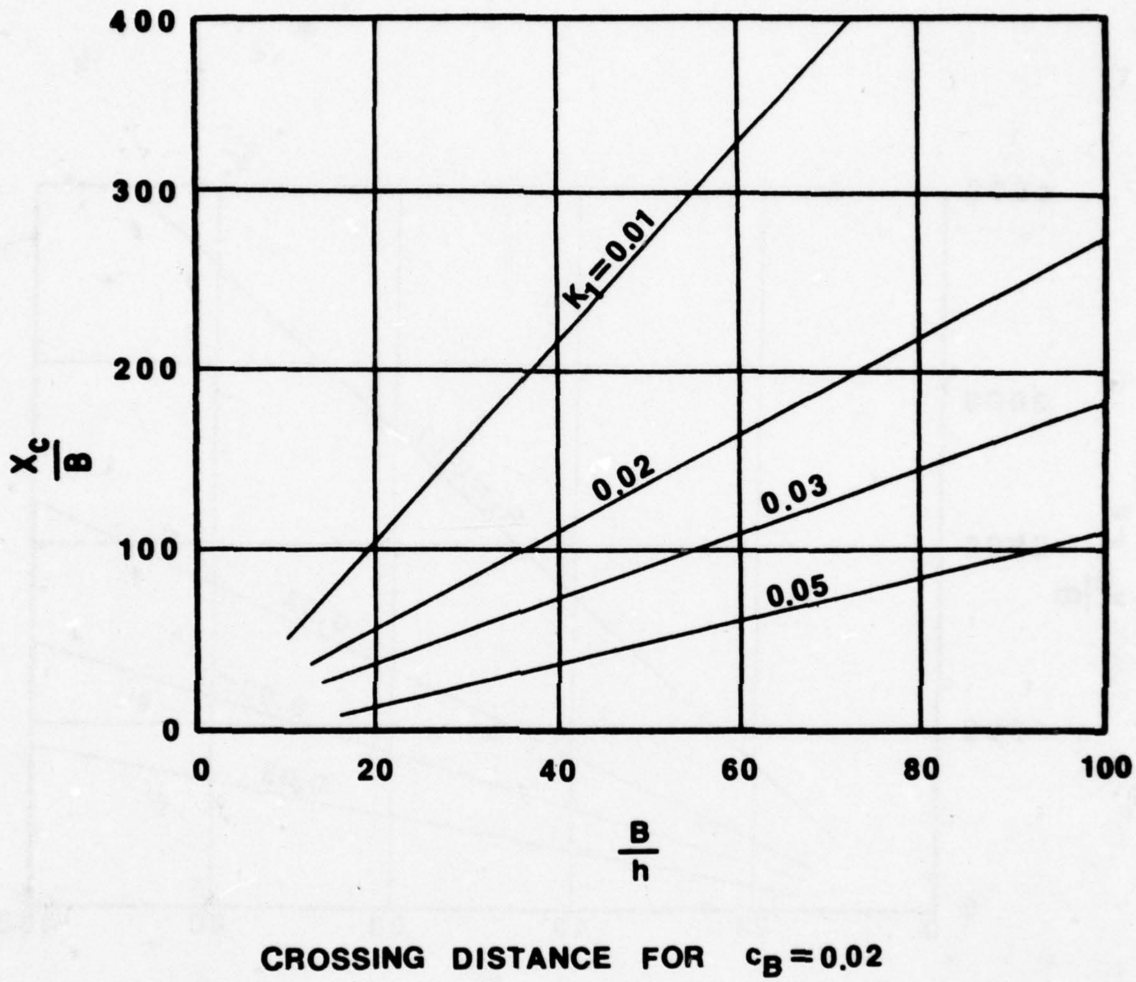


Figure 9. Crossing Distance [After Holley (23)]

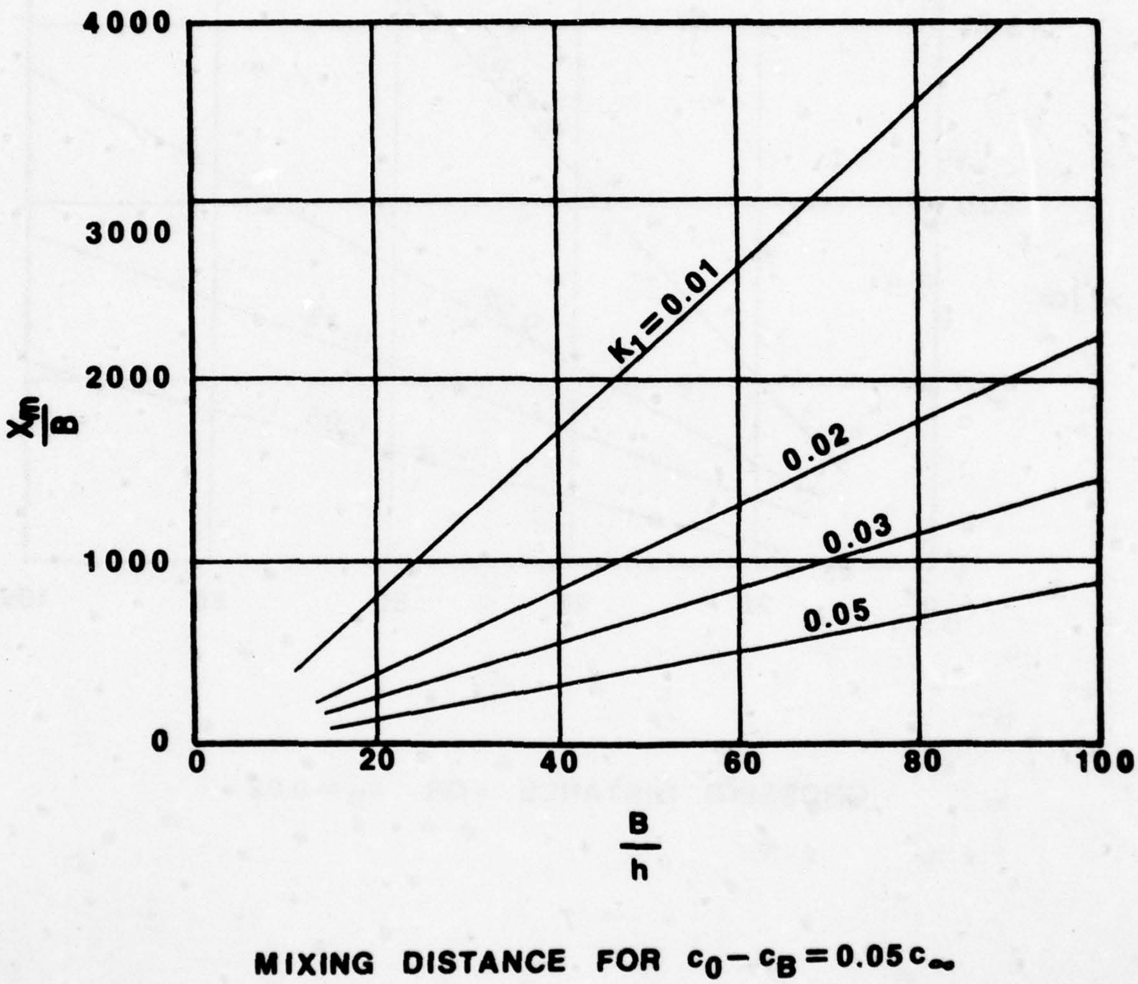


Figure 10. Mixing Distance [After Holley (23)]

Figure 10 defines complete mixing as that point where cross-sectional variation of concentration is a maximum of 5 percent. Holley, et al (18) present equations describing the curves, based on using

$$D_y = K_1 uh \tag{73}$$

in which u = mean velocity

The value of K, can be related to the α of Equation (32) by use of Equation (33). The value of u/u_* is usually between 10 and 20, and K_1 is thus usually in the range of 0.02 - 0.04. Lower K_1 values may prevail in man-made channels, and higher ones in channels with extreme bends, groins, or other geometry problems. Equations describing Figures 9 and 10 are

$$\frac{X_c}{B} = \frac{0.0543}{K_1} \frac{B}{h} \tag{74}$$

$$\frac{X_m}{B} = \frac{0.445}{K_1} \frac{B}{h} \tag{75}$$

in which X_c = crossing distance

X_m = mixing distance

both as defined above.

A range of K_1 values are illustrated in the Figures. It is interesting to note that both X_c and X_m vary in proportion to the logarithm of the assumed percentage variation selected. For example, in Figure 9, C_B = concentration at y = B and C_o = concentration at y = o. The value of X_c/B varies inversely with $\ln(C_B/C_o)$. For example, if C_B/C_o were selected as 0.01 rather than the 0.02 used, the right side of Equation (74) would have to be multiplied by $\ln(0.02)/\ln(0.01) = 0.85$.

In Figure 10, C_∞ is the completely mixed concentration, given by

$$C_\infty = \frac{Qm}{uhB} \tag{76}$$

in which Qm = total flow rate of discharged material. Values of Xm/B vary

in proportion to $\ln [(C_o - C_B)/4 C_\infty]$. As an example, if 10 percent variation across the channel were taken as the criterion, rather than the 5 percent shown, the right side of Equation (75) would have to be multiplied by $\ln(0.10/4)/\ln(0.054) = 1.26$.

It is recommended very strongly that any attempt to employ a 1-D model be checked thoroughly against the criteria presented here to assure its applicability. It is important to note that unless the non-1-D region is very short, an appropriate 2-D or 3-D model should be used up to the point where one-dimensionality occurs.

CONCLUSIONS TO SECTION III

It has been shown that selection of coefficients for diffusion models is not a simple task. The coefficients are a function of the physical site and the particular model being used.

The first step in model selection must be a review of the model, listing the averaging steps it has undergone to assure full understanding of what the coefficients in the model represent.

1. D_z Value - The simplest coefficient selection should be the vertical coefficient, D_z, which is defined as $0.067hu_*$. This may be decreased in the presence of density stratification or it may be increased if bottom irregularities are thought to increase vertical mixing. No good guidance exists on how much to increase or decrease D_z in those cases.

2. D_y Value - The transverse mixing coefficient, D_y, has a basic value of $0.15hu_*$. The biggest single factor changing this standard value is the existence of bends, although density differences can also play a major role.

In bends, the transverse velocityies created by the geometry are the main features. If a stream tube model such as that by Holly (115) is used, the transverse velocities are implicitly included and this modification to the standard value does not have to be made. In other models, however, two

separate types of adjustments may be necessary, one for local behavior in a bend and the other for longer stretches of the waterway passing through many bends. For local processes in the bend itself, the work by Chang (13) provides some guidance to the variation through the bend. For longer reaches, Chang (13), Krishnappan and Lau (19), Yotsukura and Sayre (38), and Fischer (89) all provide values. Ward (86) provides very similar values in an oscillating flow. It is important to observe that D_y never exceeds about $2hu_*$ through a series of bends unless there are other features as well. This provides an upper limit.

Stratification existing in the receiving water has not been investigated much with regard to D_y. However, Sumer (73) has shown values for D_y in unsteady, stratified flows which are also less than $2hu_*$, or the same order as values due to bends.

Prych (45) has provided the best work on mixing rates where the effluent and ambient densities differ. One should check the distance over which the density influence would be felt. Calculations inside that range should use Prych's modified values, while beyond that the density effect can be neglected.

If the discharge is into a lake or very wide water body, it may be more appropriate to use the four-thirds law [Equation (34)] for estimating D_y.

3. Values for $D_x(D_L)$ - It must first be ascertained whether averaging of velocity, etc., has occurred across the entire cross-sectional area or only vertically. In the former case, the designation D_L (longitudinal dispersion coefficient) is more appropriate. The value for D_x where only vertical averaging has been performed is usually taken from Elder's (42) work as $D_x = 6hu_*$.

If the appropriate coefficient is D_L, one must first compare the width of the water body to the expected plume width. Holley, et al (82) discuss this concept in estuaries and a similar approach could be used in rivers. If

the plume covers only a small part of the stream width, Elder's (42) value of $6hu_*$ may still be appropriate. If the plume covers a substantial portion of the stream width, then more must be known about the lateral variation. At the current time, in estuaries it is recommended that the Thatcher-Harleman relationship [Equation (57)] be used to estimate D_L, with the Holley, et al (82) methods used to estimate values for smaller plumes.

For rivers, a number of empirical relationships exist and are summarized in Section III - 3.d. One approach is to calculate D_L by all techniques and compare. The methods by Jain (67) and Fischer (66) should be given more weight because they are theoretically more sound. None, however, are excellent.

4. Conservative Estimates - There is a fairly high level of uncertainty in selecting coefficients for model use. Some of this can be alleviated by using models retaining more detail of the advective flow field. In any case where it is desired to assess potential spill impact, coefficients should be selected to provide a measure of safety. If results are still acceptable, then no further estimates are needed. If the predictions indicate a potential problem which disappears when upper limit coefficient values are used, it will be necessary to better refine the values. In general, lower coefficient values should be chosen to minimize mixing and provide conservative results. They should never be lower than the lower limits. For example, D_x should never be less than $6hu_*$.

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REVIEW OF TOXIC SPILL MODELING.(U)

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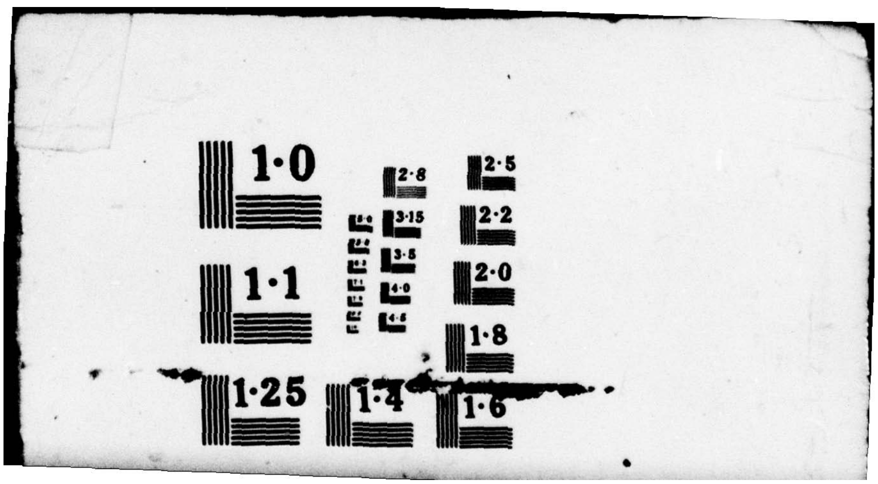
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SECTION IV

TECHNIQUES FOR SOLUTION OF DIFFUSION EQUATION

GENERAL BACKGROUND

The equation to be solved has been derived and given as Equation (11), the three-dimensional convective diffusion equation. The literature has many discussions about solution techniques for these equations, but they all fit three basic types:

Integral transform methods

Method of images

Numerical methods

Brief mention will be made later of numerical methods, but the major thrust here will be the first two techniques. This is because the Air Force needs will be much better served by analytical models which can be applied widely with a minimum of backup data required. Numerical models require much more extensive programming, user skill, and interpretation, coupled with a need for data at a much higher level than is called for in the assessment and planning modes needed by Air Force users. In fact, some of the data is often not available.

This report is not intended to be a basic text, and therefore where adequate coverage appears elsewhere, the reader will be referred there for details. Greater detail will be presented on the method of images due to the feeling that it is not adequately described elsewhere in the generally available technical literature. Probably the single best reference is the classic by Carslaw and Jaeger (102). However, Crank (103) has an excellent presentation, and Jost (104) and Monin and Yaglom (105) also present useful reviews. In reviewing the next sections, a key fact should be remembered about the convective diffusion equation. The convective diffusion equation (Equation (11) and its simp-

lified versions) is linear, in that the sum of one or more solutions to the equation is itself a solution. This is often called the superposition principle.

BOUNDARY CONDITIONS TO BE MET

The primary constraint in the solution of Equation (11) lies in the boundary and initial conditions which must be met. These will vary according to the specific case being considered, but the most general condition is the no-flux boundary. In order to assure that no material is transported past the physical boundaries of the system, there must be no transport past the air-water interface (z=0), the two lateral boundaries (y=0 and y=B, the stream width), or the bottom boundary (z=h, the stream depth). This can be expressed as $\partial c/\partial n = 0$, or the concentration profile is normal to all these boundaries. Other boundary conditions are imposed by the size and shape of the source, as well as the time distribution of the material release. In addition, initial conditions of concentration are determined by "ambient" concentrations, or at lease those existing prior to the release.

1. Solution by Integral Transform Techniques - A direct analytical solution technique exists for certain cases, using the method of integral transforms. It is somewhat difficult to use as the problem to be solved increases in complexity. It is generally true that many of the effects which are lumped into the coefficients, especially by partial averaging (see Section II) are very difficult to define due to the complexity of the solution forms. However, it provides a systematic approach to a very difficult problem and is beginning to appear more and more frequently in the technical literature, as can be seen in the review of models in Seciton V.

A full description of the integral transform technique for solution of differential equations is presented in the references cited, as well as numerous mathematical texts, including the one by Snedden (106). Cleary and Adrian (107) present a very thorough version of the solution process. They show a

two-dimensional and a three-dimensional solution with certain assumptions involved. For example, for the two-dimensional case, one finite (vertical) and one infinite (longitudinal) dimension can be transformed out of the convective diffusion equation by use of a finite Fourier transform and a complex Fourier transform, respectively. This results in an ordinary differential equation with time as the dependent variable. This equation can be integrated directly for the transformed variable which represents concentration. This variable must then be converted back to the real concentration by "inversion", i.e., by integrating by appropriately defined inversion formulae which reverse each transforming integration made initially. In this case, two integrations were used in the transform process and therefore a double inversion is required. The process is identical in three dimensions except that one more integral transform is required to remove the finite lateral dimension. Of course, one more inversion formula is required for conversion back to the real concentration.

The above description oversimplifies a complex set of operations. The complexity increases as more realistic variability in the physical parameters is allowed. For example, use of a single, constant longitudinal velocity yields simpler solutions than those suggesting more realistic cross-sectional variations. In addition, those dealing with time-varying flows are even more complex. From the standpoint of a model user, rather than a model developer, other features of the method are more important than the underlying mathematical manipulations. A key thing to remember in all model reviews is to be sure to understand the assumed flow conditions, source conditions, and boundary conditions.

The form of the solution obtained by integral transform techniques usually consists of one or more combinations of infinite series of sine and/or cosine terms. Examples will be shown later. It is worth noting that one of the

difficulties of these series is that they are very slow to converge and may therefore require a large amount of computer time. Holley, et al (18) and others (108) report this fact.

2. Solution by Method of Images - The second technique involves use of the method of images, outlined in Carslaw and Jaeger (102), Prakash (109), and Benedict (110). This method takes advantage of the superposition principle, in that the sum of a number of solutions to Equation (18) is itself a solution. As an example, consider the solution to Equation (18) obtained for an infinite medium, i.e., no boundaries exist. If this solution is written for two sources of the same strength (flowrate and concentration) at different locations, the sum of these two solutions has the characteristic that there is a plane surface midway between the two sources across which there is no transport of material, or $\partial c/\partial n = 0$, which is exactly the required condition which must exist at a physical boundary. In this example, one source is inside the real flow field and is the real source. The other is outside the physical flow field and is referred to as an imaginary, or image, source. Therefore, proper selection of locations for image sources and the resultant summation can yield a set of physical limiting planes exactly corresponding to the stream surface, bottom, and lateral boundaries. It develops that this requires infinite series of terms in the vertical and lateral directions. Inasmuch as the basic solution form contains exponential terms, the image solution is then one or more infinite series of exponential terms, versus the sine-cosine terms from the integral transform method.

The reason the infinite series becomes necessary can be seen by reviewing Figure 11, taken from Cochrane and Adrian (111). The real source is R. Image source 1 , is placed to balance the real source across the bottom boundary and yield a no-flux boundary at that location. Image source I_2 is similarly placed for the surface. However, each time an image source is placed to balance one

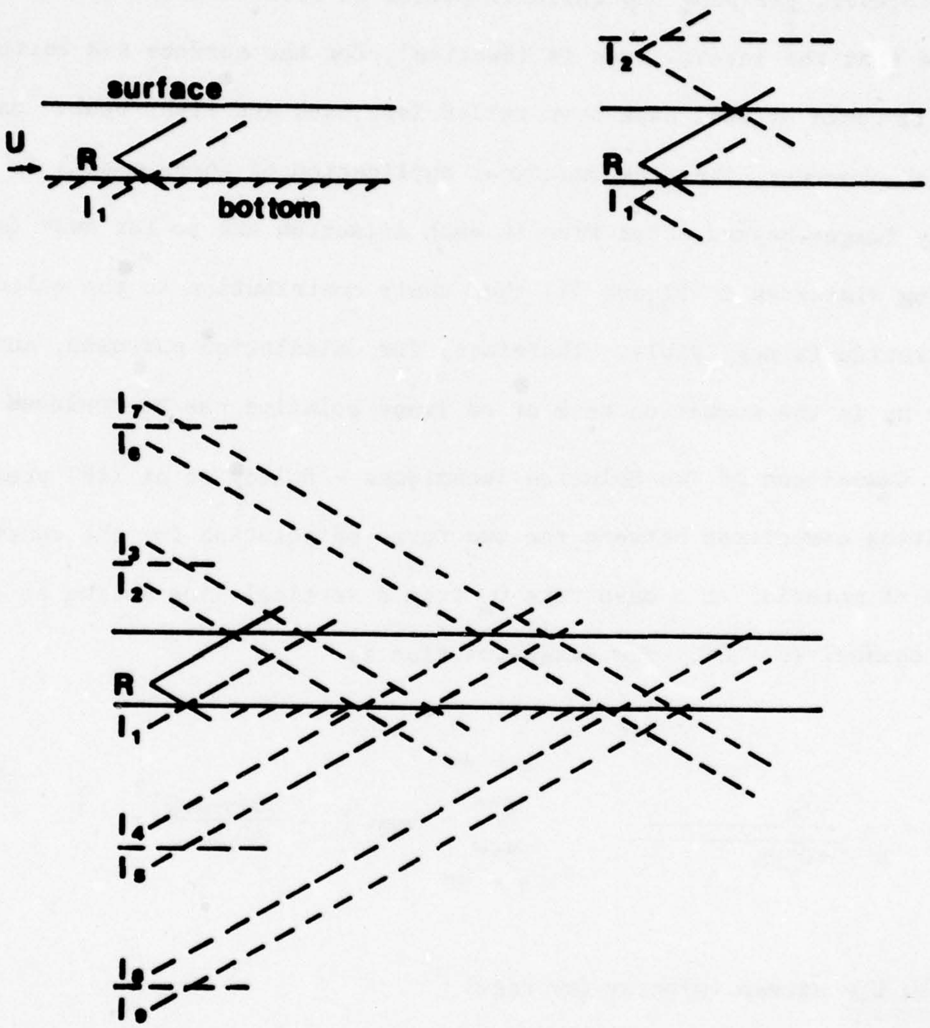

Figure 11. Schematic of Image System [After Cochrane and Adrian (111)]

boundary, it automatically unbalances (creates a net flux) at the other boundary. Hence, another one must be placed to offset that effect. For example, I_3 is placed to offset I_1, and I_4 to offset I_2. Obviously, this process continues forever, yielding the infinite series in both directions. It should be noted that the lateral case is identical, for the surface and bottom in Figure 11 could as well have been called left bank and right bank. Sayre (112) has noted, however, that the practical application of these models is such that any images beyond about five in each direction are so far away (see the expanding distances in Figure 11) that their contribution to the calculated concentration is negligible. Therefore, for calculation purposes, any ∞ showing up in the summation term of an image solution can be replaced by 5.

3. Comparison of Two Solution Techniques - Holley et al (18) present an interesting comparison between the two forms of solution for the continuous release of material at a mass rate Q_m from a vertical line source at one edge of the channel ($y = 0$). The image solution is

$$C = \frac{Q_m}{h\sqrt{\pi D_y U x}} \sum_{n=-\infty}^{n=+\infty} \exp\left[-\frac{U(y-2nB)^2}{4D_y x}\right] \tag{77}$$

in which U = stream velocity (average)

The integral transform solution is

$$C = \frac{Q_m}{hBU} + \frac{2Q_m}{hBU} \sum_{n=1}^{\infty} \frac{\cos\frac{n\pi y}{B}}{(1+\alpha_n)^{1/2}} \exp\left\{\frac{Ux}{2D_y}\left[1-(1+\alpha_n)^{1/2}\right]\right\} \tag{78}$$

in which

$$\alpha_n = \left(\frac{2D_y n\pi}{uB}\right)^2 .$$

The two solutions given by Equations (77) and (78) are numerically equivalent, as they should be. However, Holley et al (18) note that Equation (77) requires only a few terms of the series to converge for small x, while Equation (78) requires only a few terms at large x. Kuo (113, 114) notes that the transform solution may take in excess of 100 loops to converge. While this can be accomplished on the computer, it in less efficient. In addition, the image summation process makes it easier to see the effect of boundaries.

DESCRIPTION OF BASIC MODEL BUILDING

This section is devoted to describing the process by which various source conditions are simulated by use of the superposition principle. The term source refers to the physical location of the injection of the spilled material into the receiving water, as well as to its rate of input with time. The physical location of the spill is frequently treated as a point, having no physical dimensions. However, if reason exists to believe that the spilled material quickly occupies some larger volume of the receiving water, the point source solution can be integrated over that space to yield the correct solution. The initial volume of interest here is the volume or space occupied by the spilled material as it undergoes initial mixing upon entering the water prior to beginning to be mixed by processes of ambient diffusion and dispersion. For example, a tankful of liquid spilled from a truck might be assumed to occupy a finite volume immediately upon entering the water. Material leaking from a barge might seem to issue from a finite size plane source, or, in the case of a long, thin crack, a line source of material.

Common categories of simplified sources assumed for models include the following:

Point source: located at x_o, y_o, z_o

Vertical line source: located at $x = x_o$, $y = y_o$

from $z = z_1$ to $z = z_2$

Horizontal line source: located at $x = x_o$, $z = z_o$, extending from $y = y_1$ to $y = y_2$

Plane source: covering part of the cross-sectional area of the stream = located at $x = x_o$, extending from $y = y_1$ to $y = y_2$ and from $z = z_1$ to $z = z_2$

Volume source: covering a finite stream volume - extending from $x - x_1$ to $x = x_2$, $y = y_1$ to $y = y_2$, and $z = z_1$ to $z = z_2$

The most realistic source from a physical standpoint is the volume source. Any material spilled into the water enters into a finite stream volume. These spills may include material falling over a bridge from a truck accident, leaking from a damaged barge, entering the stream by way of a storm drain, or other means. The difficulty lies in defining the size of the finite volume source over which the spilled material is distributed. Work is planned to define this by using jet entrainment theory, but only judgement is available now. However, at distances sufficiently far from the source the concentration predictions look the same regardless of the initial source configuration. This is because the mixing has masked the original conditions. No firm guidelines exist now, however, as to the distance downstream one must go for the point source to be a totally acceptable source approximation. For the time being, it is suggested that the best estimate possible be made, realizing that the influence of errors in selection will only be important near the spill location.

The time rate of the release during a spill may range from instantaneous (all material enters water at one instant of time) to continuous (material continues to enter the water at the same rate for an indefinite time). In between these extremes lie many possible spill histories representing finite

times of spills. For example, a spill of material from a truck might be assumed to last 10 minutes, with the rate of flow varying over that time and gradually decreasing to zero. However, an undetected storage tank leak which flowed into a storm drain and then into the stream might continue to flow for a number of hours at a fairly constant rate. All of these cases can be treated by integrating the instantaneous source solution over the time from beginning to end of the spill. Numerically, this integration can be achieved by replacing the spill by a series of instantaneous releases yielding the same total release rate and spaced closely enough in time to adequately approximate the uninterrupted spill.

1. **Basic Point Source Equations** - It is necessary to have a point source solution in order to integrate it over time or space. Appropriately, the final equation solution must include both correct source conditions and any image or boundary terms. The solution can be compiled by integrating the point source solution for an infinite flow field to obtain the required source and then imposing the method of images to meet the boundary conditions. On the other hand, it is also possible to include the images in the point source solution first and then to integrate. The former viewpoint will be employed here, as it seems easier to visualize, e.g., that a series of imaginary plane sources are needed to balance a real plane source. The point source solution for both continuous and instantaneous discharges can be found in numerous references. The infinite field solutions are given first.

Instantaneous Point Source:

$$c(x,y,z,t) = \frac{M \exp \left| - \frac{(x-ut-x_o)^2}{4D_x t} \right|}{8\pi t \sqrt{\pi D_x D_y D_z}} \cdot \exp(-\lambda t)$$

$$\cdot \exp \left\{ - \frac{(y-y_o)^2}{4D_y t} \right\} \exp \left\{ - \frac{(z-z_o)^2}{4D_z t} \right\} \tag{79}$$

in which t = time measured from t_o, the time of release

M = total volume of tracer material released = $C_o V_o$

x_o, y_o, z_o = coordinates of point of release

V_o = total volume released

λ = rate of decay, dimensions 1/time

Continuous Point Source:

$$c(x,y,z) = \frac{c_o Q_o \exp(-\lambda x/u)}{4\pi x \sqrt{D_y D_z}} \exp\left\{-\frac{(y-y_o)^2}{4D_y x/u}\right\}$$

$$\cdot \exp\left\{-\frac{(z-z_o)^2}{4D_z x/u}\right\} \tag{80}$$

in which c_o = initial discharge concentration

Q_o = rate of discharge of material

Several important features should be noted immediately. Both solutions assume that all transverse and vertical velocities are zero (v=w=o). Also, the solutions are for cases where only one sink term appears, that of a first order reaction given by the expression

$$\text{sink} = \lambda c \tag{81}$$

This term appears in the diffusion equation preceded by a negative sign, as it is a sink. Other source or sink terms will naturally change the basic solution. The interest here is in selection of the simplest form to assure ease in understanding the model formulation process. One other point of interest lies in the failure of D_x to appear in the steady state Equation (80). This is consistent with the assumption that the longitudinal dispersion influence is negligible in steady flow cases, but its full significance will be explored later in this section and again in Section VI.

It should also be noted that Equations (79) and (80) are for unbounded flow fields. Application of the method of images yields the following results for

a flow field with finite width and depth.

Unsteady Point Source - Bounded Field:

$$c(x, y, z, t) = \frac{M \exp(-\lambda t) \exp\left\{-\frac{(x - ut - x_o)^2}{4D_x t}\right\}}{8 \pi t \sqrt{\pi t D_x D_y D_z}}$$

$$\sum_{m=-\infty}^{m=+\infty} \sum_{n=-\infty}^{n=+\infty} \left[\exp\left\{-\frac{(y - y_o - 2nB)^2}{4D_y t}\right\} + \exp\left\{-\frac{(y + y_o - 2nB)^2}{4D_y t}\right\}\right]$$

$$\left[\exp\left\{-\frac{(z - z_o - 2mh)^2}{4D_z t}\right\} + \exp\left\{-\frac{(z + z_o - 2mh)^2}{4 D_z t}\right\}\right] \quad (82)$$

Continuous Point Source - Bounded Field:

$$c(x,y,z) = \frac{c_o Q_o \exp(-\lambda x/u)}{4 \pi x \sqrt{D_y D_z}}$$

$$\cdot \sum_{n=-\infty}^{n=+\infty} \left[\exp\left\{-\frac{(y - y_o - 2nB)^2}{4 D_y x/u}\right\} + \exp\left\{-\frac{(y + y_o - 2nB)^2}{4 D_y x/u}\right\}\right]$$

$$\cdot \sum_{m=-\infty}^{m=+\infty} \left[\exp\left\{-\frac{(z - z_o - 2mh)^2}{4D_z x/u}\right\} + \exp\left\{-\frac{(z + z_o - 2mh)^2}{4D_z x/u}\right\}\right] \quad (83)$$

2. Spatial Integration for a Source - Use of the superposition principle to define a source of any spatial extent can be visualized easily. Consider a discharge assumed to originate over some space. Visualize that source as composed of an infinite number of point sources. Thus, at any point in space and time, the concentration can be calculated by summing up the contribution at that pojnt due to each of the point sources comprising the spatial

source. As the spatial source is a continuum, this summation is the same thing as integrating the solution over the given spatial domain which defines the source. In this integration process, the error function will frequently appear, noted as erf and defined as

$$\mathrm{erf}\ (a) = \frac{2}{\sqrt{\pi}} \int_{o}^{a} e^{-t^2}\ dt \qquad (84)$$

in which t = dummy variable.

3. **Time Integration for Unsteady Source** - The discharge may have many types of time histories. For the purposes of this discussion, unsteady implies any source other than one which continues at a constant rate long enough to achieve steady-state conditions at any downstream point of interest. Thus, for example, a discharge which occurs at a steady rate for a finite time and then drops to zero before a steady value of concentration is reached at downstream locations of interest, is classed an unsteady source.

The unsteady source can be visualized as composed of an infinite string of instantaneous releases. Note that these could be instantaneous point sources, plane sources, or whatever other spatial character is assumed to represent the source. The concentration at any given point in time and space is then found by summing up the contribution due to each of these instantaneous releases, or integrating over time. To cover the most general discharge history, this integration will ordinarily be done numerically. Then the discharge is assumed to be adequately represented by a series of instantaneous releases at finite time intervals. Obviously, the time interval selected must be short enough so that the difference in predicted concentration between that for a continuous release and that for a finite-interval series is negligible. No firm guidelines exist now for selection of the time interval. However, intuitive reasoning and experience in requirements for unsteady flow calculations

in open channels indicate that at the least the interval between slugs released should be very small compared to the travel time to the point at which concentrations are calculated. Probably the best approach for any given case at current is to experiment using several time increments and note the size of increment below which no significant change in predictions occur. Then use that increment. Note that use of a smaller increment than necessary increases calculation time, while use of a larger increment leads to inadequate description of the physical case.

Once the time interval is selected, the material released at each time can be determined from

$$M(t) = \int_{t}^{t+\Delta t} C_o \, Q(t) \, dt \qquad (85)$$

in which $M(t)$ = volume of tracer released over time Δt and therefore assumed as instantaneous release

$Q(t)$ = rate of effluent flow as function of time

C_o = concentration of tracer in effluent

Of course, the integration suggested in Equation 4.9 may well be carried out numerically. In deed, for the short time intervals used in such calculations, the average flow could be used over that interval, yielding

$$M(t) = C_o \, \overline{Q}_o \, \Delta t$$

in which $\overline{Q}_o$ = average effluent flow rate over time interval Δt

Holly (115) presents a review of the superposition principle, and Sayre (112) presents a very thorough discussion. The main thing to recall here is that virtually any source can be derived by considering it to be composed of numerous individual releases in space and/or time.

4. Influence of Longitudinal Dispersion - While a more lengthy discussion will be presented later (Section VI, it is beneficial to look at the longitudinal dispersion contribution now, especially since it is frequently neglected in the basic steady-state building blocks, e.g., Equations (80) and (83). It may be helpful first to note the solution to the longitudinal dispersion (one-dimensional) equation first. It can be written (10, 115) as the following.

Instantaneous Plane Source - One-Dimensional:

$$c(x,t) = \frac{M}{2A\,(\pi D_L t)^{1/2}} \exp\left\{-\frac{(x - ut - x^o)^2}{4D_L t}\right\} \tag{86}$$

in which A = cross-sectional area of flow

This is a solution to Equation (18) for a single, constant mean velocity, u, and longitudinal dispersion coefficient, D_L. Discharge is from a plane source covering the entire cross-sectional area of the channel, or a discharge assumed to have become completely mixed across the section. Recall the subsection on applicability of the one-dimensional equation. The solution shown in Equation (86) is a Gaussian, or bell-shaped, curve which flattens and spreads out as it moves down stream. The peak moves at about the mean travel velocity of the stream, distorted somewhat by dispersion. This characteristic is the reason many dye studies are used to obtain so-called time-of-travel data. A very great deal of attention has been given to evaluation of D_L for use in Equation (86). Because it frequently oversimplifies the problem too much, this equation is being somewhat displaced as better analytical tools and physical understanding develop. However, as it may still provide useful preliminary estimates in some cases and even be appropriate in small streams, some discussion is in order here.

Godfrey and Frederick (64) observed that data indicated that Equation (86) generally predicted a rising limb (of the concentration versus time curve) which was too flat and a falling limb which was too steep. Data showed a

tendency for there to be a very long "tail" on the concentration vs, time curve, implying that some material lagged quite far behind. A number of workers have attempted to treat the process by considering so-called dead zones or separation zones to exist. These zones are attached to the main channel and may include small embayments, shallow overbank regions, lee regions of a bend, or protruding structures, and slow moving regions near the stream bed caused by dunes or submerged structures. Material is assumed to move into these dead zones and then to very slowly reenter the main channel flow, thereby spreading the cloud of discharged material far more than by mere shear-induced dispersion. Hays, et al (116) present a solution for the coupled main flow dispersion equation and side channel-main channel exchange equation. There is some question as to the need for this level of complexity in preliminary assessments, considering especially all the uncertainties inherent in use of the 1-D equation and selection of D_L. It is clear, however, that these dead or separation zones exist and must be ultimately considered in final selection of models and coefficients.

Frenkiel (117) and others have integrated the equivalent of Equation (11) with $v = w = o$ and neglecting the longitudinal turbulent diffusion term (the e_x term). This yields the steady-state Equation (80). It has generally been assumed that this deletion is valid. Thoman (39) notes that if the discharge varies with a period of one week or less, the longitudinal term should be retained in many 1-D, longitudinal dispersion calculations. Dobbins (118) has shown by sensitivity testing that for steady river flows within practical ranges of flows and sizes, longitudinal dispersion is unimportant in a 1-D dissolved oxygen model. It must be recalled that if either the effluent flow rate or the receiving water flow rate is unsteady, longitudinal dispersion cannot be neglected.

Sayre and Chang (10) present an instructive solution for the case of a

two-dimensional mixing problem from a vertical line source extending from the water surface to the stream bed. The discharge is into a laterally unbounded water body. Integration of the solution for an instantaneous vertical line source yields

$$C(x,y) = \frac{Q_o\ c_o}{2\pi h\sqrt{e_x\ e_y}} \cdot \exp\left(\frac{ux}{2e_x}\right)$$

$$\cdot K_o\left[\frac{u}{2e_x}\left(x^2 + \frac{e_x}{e_y}\ y^2\right)^{1/2}\right] \tag{87}$$

in which K_o = modified Bessel function of second kind, order zero

The coordinate origin (x and y) is assumed to coincide with the source location here.

Sayre and Chang (10) note that if

$$\frac{e_x}{e_y}\ \frac{y^2}{x^2} \ll 1 \text{ and } x \gg \frac{2e_x}{u}$$

then Equation (87) converges to

$$C(x,y) = \frac{Q_o\ c_o}{2hu\,(\pi x e_y/u)^{1/2}}\ \exp\left(-\frac{uy^2}{4e_y x}\right) \tag{88}$$

Equation (88) is equivalent to integrating Equation (80) from z = 0 (surface) to z = h (stream bed). One can then view the inequalities shown as a means of estimating, at least for this source condition, the distance downstream which must be reached to assure that neglect of the longitudinal term is adequate. For practical open channel flows, the two conditions described are met except for very near the source, and thus neglect of the longitudinal term is appropriate for continuous discharges (10). However, recall the discussions in Section II on the effects of partial averaging on coefficient values. If a single, cross-sectional average velocity is used, then e_x should be replaced

by D_L, for this coefficient now includes all the behavior due to cross sectional variation of velocities. In this case, the length to be attained may be more significant. Calling L_n the distance to the point where D_L effects are negligible for this continuous vertical line source discharge,

$$L_n >> \frac{2D_L}{u} \tag{89}$$

in which D_L can be replaced by D_x if only vertical averaging has occurred

A quick look at representative values for $2D_L/u$ may help. In the Missouri River, Yotsukura, et al (54) report values for D_L as high as 30,000 ft^2/sec, with velocities (u) ranging from 3.9-6.0 feet/second . Using their average u over the reach of 5.34 feet/second and average D_L of 16,000 ft^2/sec, one can see from Eqn. (89) that L_n must be greater than about 6,000 feet. On the other hand, a small stream, the Comite River (width = 41 ft) was reported by McQuivey and Keefer (66) to have a $D_L = 75\ ft^2/sec$ with u = 1.02 feet/second . Eqn. (89) yields a value of 150 feet, for L_n, which is essentially negligible.

Criteria do not currently exist for other source conditions. However, Eqn.(89) is a reasonable means of attaining a first estimate of L_n when concentration values quite near the source are desired. The purpose of these last paragraphs has been to illustrate the fact that while the neglect of longitudinal mixing for continuous discharges is generally valid, there is likely to be a region near the source where this is not so.

NUMERICAL MODELS

All the solutions to the diffusion equation discussed thus far are analytical solutions to the differential equation itself. It may often be necessary or more efficient to use a computer to numerically evaluate series or other terms appearing in the equations, but there is still an explicit equation for the concentration. On the other hand, there are a number of numerical models

which have been developed. These models solve a set of equations which serve as an approximation to the actual differential equation, rather than the differential equation itself. These models are often finite difference or finite element models. A discussion of the details of such models is beyond the scope of this report. However, some knowledge of their utility and status is helpful.

This report places its primary emphasis on analytical solutions. It is believed that, especially considering many uncertainties already described, many of the assessment and planning problems which must be addressed with spills of toxic materials can be adequately addressed with analytical models with a much smaller expenditure of time and money than with numerical models. The data input requirement for many numerical models can be substantial, requiring time for collection and coding for computer use. In addition, the same uncertainty about physical processes which exists in analytical solutions is a limiting factor with numerical models. However, there are some strong points to be considered with numerical models. In addition, a two-level procedure may be possible in many assessments. The first level uses an analytical solution to estimate impact of a spill or other discharge. If no problem seems to exist in the receiving waters, then no further approach is needed. If, however, a potential problem appears (in terms of excessive concentrations or exposure times), then a very critical review of the water body and discharge configuration needs to be made. Several questions need to be asked, including these:

- Does the analytical model seem to incorporate all pertinent aspects of the physical system, e.g., bends, buoyancy, unsteadiness, etc ?
- If there seems to be possible inadequacy in the analytical model, is there a numerical model which offers any improvement?

These questions demand an understanding of the physical system. The fact that a numerical model exists does not automatically make it better

than an anlytical model. Improper understanding which leads to improper input could make the numerical model give horrible results. In addition, if important physical processes (tidal velocities, etc.) are omitted from the numerical model, then some real question exists as to any advantage in its use. One important advantage of analytical solutions lies in the visibility of all the pertinent parameters in the equation and the ability to more clearly see how they affect the results.

1. Advantages of Numerical Models - There are some areas, as discussed by Holly (115), in which analytical models have some difficulties. In general, most of these difficulties relate to geometry. In streams of non-rectangular slope, the use of the image method is unwieldy if not impossible. Prakash (109) presents a result for a point source in a trapezoidal channel which is very lengthy. What is equally limiting is that most of the solutions require an assumption of longitudinal uniformity of the flow. This is equivalent to requiring an unchanging channel section. Obviously, one of the main features of natural channels is the non-uniformity they exhibit. The stream tube models proposed by Yotsukura and his colleagues provide an increased ability to incorporate unusual cross-sectional geometry. However, existing analytical solutions to these models assume longitudinally uniform flow and a constant diffusion coefficient. Fischer's routing method (54, 63) allows for arbitrary stream geometry and velocity districution for a steady injection of tracer. Fischer's method is not a solution to an analog of the differential equation, but rather to what is believed to be the set of physical processes involved in the mixing process.

It is possible to incorporate a good deal of advective information into numerical models. In fact, the water quality diffusion model can be coupled with a hydrodynamic model which predicts flow depth and velocity as a function of space and time. These predicted depths and velocities can then be used in

the numerical model of the diffusion equation. An alternative is to use measured depth and velocity values as input. Earlier sections have pointed out the value of retaining as much advective detail as possible. Despite the numerous advances in numerical modeling of unsteady hydrodynamics, there are still many shortcomings.

2. Difficulties with Numerical Models - Reference has already been made to the complexity of these models, the expense, and the data requirements. Three-dimensional models dealing with thermal discharges frequently use several hours of high-speed computer time to generate a solution for a single discharge condition (119). In addition Cunge (120) notes the extreme difficulty with adapting even well-documented models to one's own cases.

There is another feature of numerical techniques which is very important. It goes under various names, often something like numerical dispersion. This is apparent diffusion or dispersion which occurs with no physical basis but is rather a consequence of the numerical computation method. A related problem is the ability of the model to handle sharp changes in geometry, sudden flow changes, or other such changes. That is, are these perturbations damped as they are in the physical system, or do they propagate and induce numerical errors. Since most users of numerical methods will not investigate these questions very deeply (if at all), but will merely use the model, these questions are very important. If the model is not well cast and used carefully, it could produce quite erroneous results which nontheless may be difficult to detect if the physical situation is complex. In fact, it is really better when one of these models becomes unstable and predicts unbounded results (e.g., extremely large velocities, negative concentrations, etc.) for then the user can easily see something has gone amiss.

Sound theoretical approaches to the stability and convergence of numerical solutions have begun to appear, as typified by the work of Dailey and Harleman (78),

Holly (115), and Liggett and Cunge (121). Much remains to be done in this area, but any numerical model to be employed should, at the least, have some criteria for time and distance steps to assure stability and minimize propagation of perturbations.

3. Status of Numerical Models - At the outset, it should be observed that the number of models available is large and grows larger each year. Any attempt to provide an exhaustive list would be foolish and probably out of date soon. A few key works in each main area of interest will be identified, and some brief feel for the status will be given. More thorough reviews can be found in Liggett and Cunge (121), Gray, et al (122), and others. A major impetus to numerical transport calculations has come from the concern over heated water discharges, and Jirka, et al, (95) Dunn, et al (119), and NRC (123) discuss these models.

In general, the stage of advancement of numerical models increases dramatically as the dimensionality decreases (from 3-D to 2-D to 1-D). Three-dimensional models are least well developed at this time. They not only require exorbitant computer times (up to 10 hours in some cases) for a single steady state simulation, but really do not provide any improvement in predictability. This may change in the future as understanding of the physical mechanisms increases.

Two-dimensional models have received much attention, and a number of good models exist. Consider first bodies such as embayments, lakes, etc., and then rivers. The work of Leendertse and co-workers for Rand Corporation (123-127) must be mentioned first. It represented pioneering work and is the best available documented model. In fact, the excessive documentation prompted Cunge (120) to select the Leendertse model for review. Difficulties in its testing and use were reported, and Cunge notes that much greater problems in implementation could be expected for cases where less detailed documentation was given.

Fischer (128) adapted Leendertse's model and used it in an embayment. These two-dimensional models assume fully mixed conditions prevail in the vertical direction.

Some two-dimensional numerical models applicable to spills in rivers have been developed. Rood and Holley (129) studied dissolved oxygen dynamics in a prismatic channel based on Holley's (23) modification of Siemons' (130) finite difference diffusion model. A very promising model has been developed by Holly (115) to compute both steady-state and time-dependent depth-averaged mixing of a conservative, neutrally-buoyant pollutant in a steady but non-uniform channel flow of arbitrary cross-section. The main limitations here lie in the steady river flow and conservative substance. In addition, substances such as hydrazine are not likely to be neutrally buoyant immediately. In light of what has been said in earlier sections about the distances required to achieve 1-D conditions, the most profitable area for numerical modeling of diffusion processes appears currently to be the 2-D case.

A special kind of two-dimensional case is represented by the stream tube models, used for non-conservative substances such as heat by Yotsukura and Sayre (38), Jackman and Yotsukura (131), and documented by Bauer and Yotsukura (132).

The one-dimensional case is by far the best handled. Lee and Harleman (133) developed a useful finite-difference model. Later work by the MIT group with real-time, 1-D, unsteady flows has developed a finite element model which is very versatile, dealing with salinity intrusion (75, 76), general water quality problems (78), temperature (77), and nitrogen dynamics (134). Mathematical models and users manuals are available for these cases. There are others who have applied numerical techniques to solve the 1-D non-tidal advective equation [Equations (26) or (27)]. These seem of limited interest now that models such as those from MIT exist which do incorporate the time-

varying advective terms into the model.

4. Summary on Numerical Models - This discussion has been deliberately brief. It is believed that numerical models will play a secondary role to analytical models at the current time for most planning and assessment functions. However, there are numerous advantages to well-formulated numerical models which have been established to minimize numerical dispersion. These relate primarily to the ability to handle changing and arbitrary channel geometry and any flow history. It is believed that a 2-D model similar to that by Holly (115) is a step in the right direction and deserves consideration as a potential tool in spill evaluation. The relative merits of this type of model will be further discussed in Section V. It is worth understanding that there is some real potential for use of 2-D models. If a truly 1-D situation exists, numerous well-documented numerical models exist; however, many cases will not be amenable to a 1-D analysis.

In short, numerical models currently existing are probably not the best choice for analysis of spills due to their expense, difficulty of operation, and data requirement. However, development of 2-D numerical model with proper sources and sinks could be an important tool for (a) more detailed analyses where potential problems warrant it, (b) incorporating more complex geometry into the solution, and (c) linking with analytical models describing initial mixing and three-dimensional mixing regions.

CONCLUSIONS TO SECTION IV

Solutions to the convective-diffusion equation can be made in two basic ways: analytical techniques and numerical methods. It is believed that analytical models more readily fit the assessment needs of the Air Force, although two types of numerical models are noted as potentially useful in certain cases. The, first of these are the 1-D models, especially in estuaries, where unsteady velocities are included. The second would be 2-D river models.

Analytical solutions can be achieved either by the method of integral transforms or the method of images. The two methods yield similar results. It is a matter of personal preference as to which one to use. Both enable inclusion of finite boundaries, an essential feature of any diffusion solution.

It can be expected that longitudinal dispersion has an effect which fades with distance when the discharge is continuous at the same rate. A preliminary criterion is presented by Sayre and Chang (10) which enables estimation of the initial length when the D_L term is important. Beyond that distance, the effects of longitudinal dispersion are negligible for continuous discharges into steady receiving waters. For unsteady discharges or receiving water flows, the influence of longitudinal dispersion is considerably more pronounced.

SECTION V

AVAILABLE MODELS

INTRODUCTION AND SELECTION CRITERIA

It has already been noted that new models (or revisions of old models) appear almost monthly in the technical literature. Therefore, the intention of this section is to select models representative of the types of models and solution techniques. Those selected will be chosen on the basis of versatility, their ability to represent other similar solutions which have or will appear, and in some instances for instructive purposes. On the last point, for example, some solutions for other than uniform velocity fields will be presented in order to investigate the effect on mixing. The omission of a model from those discussed does not preclude its being valuable.

As the models are reviewed, it is perhaps well to keep in mind the items needed in a model which might be used to describe a spill of hydrazine or other hazardous materials.

1. Ability of handling any time history of discharge, from instantaneous to continuous.

2. Ability to simulate finite size sources.

3. Ability to incorporate tidal advection in estuaries.

4. Coefficients which are well-defined as to their meaning, enabling more intelligent selection.

5. In addition to number 2, be easily interfaced with some model describing initial mixing.

6. Include source and sink terms to enable description of chemical and biological decay, plus other mechanisms.

7. Clearly allow boundary influences to be felt.

8. Be easy to use.

YEH AND TSAI TIDAL 3-D MODEL

Yeh and Tsai (135) have presented a very comprehensive solution by the integral transform technique. It offers versatility and describes a tidal flow system. As will be seen, however, there are some questions as to the coefficient selection procedure.

Equation (11) is used, assuming the following:

1. $v=w=o$
2. u = the mean velocity
3. The ΣS term is written as

$$\Sigma S = -k_1 c - r_2 - r_3 + S(x,y,z,t) \tag{90}$$

in which k_1 = first-order decay coefficient (units: 1/time)

r_2, r_3 = substances decomposed and generated, respectively, per unit volume per unit time

S = artificial source function

Yeh and Tsai (135) assume these forms for r_2 and r_3:

$$r_2 = k_2\, c + b \tag{91}$$

$$r_3 = k_3\, (c_5 - c) \tag{92}$$

in which k_2 = decomposition coefficient

b = that part of decomposition due to other agents

k_3 = generation coefficient

c_5 = threshold value of c above which no generation is possible

In the case of conservative discharges and thermal discharges, $k_1 = k_2 = k_3 = b = o$. For oxygen, $k_2 = 0$ and b is proportional to BOD; r_3 = rate of reaeration; coefficient; and c_5 = saturation value of oxygen. For other materials, appropriate values must be determined.

The velocity function chosen by Yeh and Tsai (135) is a sinusoidal, tidal variation, given by

$$u = U_f + U_{max} \sin \omega(t + \delta) \tag{93}$$

in which U_f = velocity due to freshwater flows

U_{max} = amplitude of tidal velocity component at maximum

ω = frequency

δ = phase lag (time) between discharge time and slack water

The modified Equation 2.10 is solved subject to these conditions.

Initial and Boundary Conditions:

$$c = o \quad \text{for } t \leq o \tag{94}$$

$$D_y \frac{\partial c}{\partial y} = o \quad \text{for } y = o \tag{95}$$

$$D_y \frac{\partial c}{\partial y} = o \quad \text{for } y = B \tag{96}$$

or

$$c = o \quad \text{for } y = \infty \tag{97}$$

$$D_z \frac{\partial c}{\partial z} - K_1 c = K_2 \quad \text{at } z=0 \tag{98}$$

$$D_z \frac{\partial c}{\partial z} = 0 \quad \text{at } z=h \tag{99}$$

$$c \text{ bounded} \quad x = \pm\infty \tag{100}$$

in which $K_1 = K_2 = o$ for conservative discharges

$K_2 = 0$ and $K_1 = K_e/\rho c_p$ for heated discharges

K_1, K_2 both nonzero for non-conservative material

K_e = surface heat exchange coefficient

ρ = water density

c_p = specific heat

Note that Equations (96) and (97) are alternative conditions. Equation (96) describes a no-flux boundary for a finite flow field, while Equation (97) scribes the condition when no far boundary exists. These two cases will be called Case A and Case B here, where Case A might be for tidal rivers and Case B for discharges into large embayments, estuaries, lakes, or the open coast.

Also observe that if U_{max} is made zero in Equation (93), then this becomes the case of a unidirectional, steady flow.

Only a few representative solutions will be presented here, although they cover the basic ones needed anyway. Many of the other source conditions present have little physical significance. More details of the solution technique are presented by Yeh (136). Yeh and Tsai (135) presented no solutions for the non-conservative case. Figure 12 shows the basic coordinate system used here and in the remaining discussions unless otherwise specified.

Point source at (x_s, y_s, z_s)

$$c = \int_o^t Q_o\, c_o\, X_1\,(x,\, t)\cdot Y_1(y,t) Z_1(z,t)\, dt_o \tag{101}$$

Line source parallel to z axis (vertical line source)

at $x = x_s$, $y = y_s$, from $z = z_1$ to $z = z_2$

$$c = \int_o^t \frac{Q_o\ \ c_o}{(z_2 - z_1)} X_1(x,t)\cdot Y_1(y,t) Z_2(z,t)\, dt_o \tag{102}$$

Plane source perpendicular to x axis; located at $x = x_s$, from $z = z_1$, to $z = z_2$ and $y = y_1$ to $y = y_2$:

$$c = \int_o^t \frac{Q_o c_o}{(y_2 - y_1)(z_2 - z_1)} \cdot Y_2(y,t) Z_2(z,t)\, dt_o \tag{103}$$

Volume source from $x = x_1$ to x_2; $y = y_1$ to y_2; $z = z_1$ to z_2

$$c = \int_o^t \frac{Q_o c_o}{(x_2 - x_1)(y_2 - y_1)(z_2 - z_1)}$$

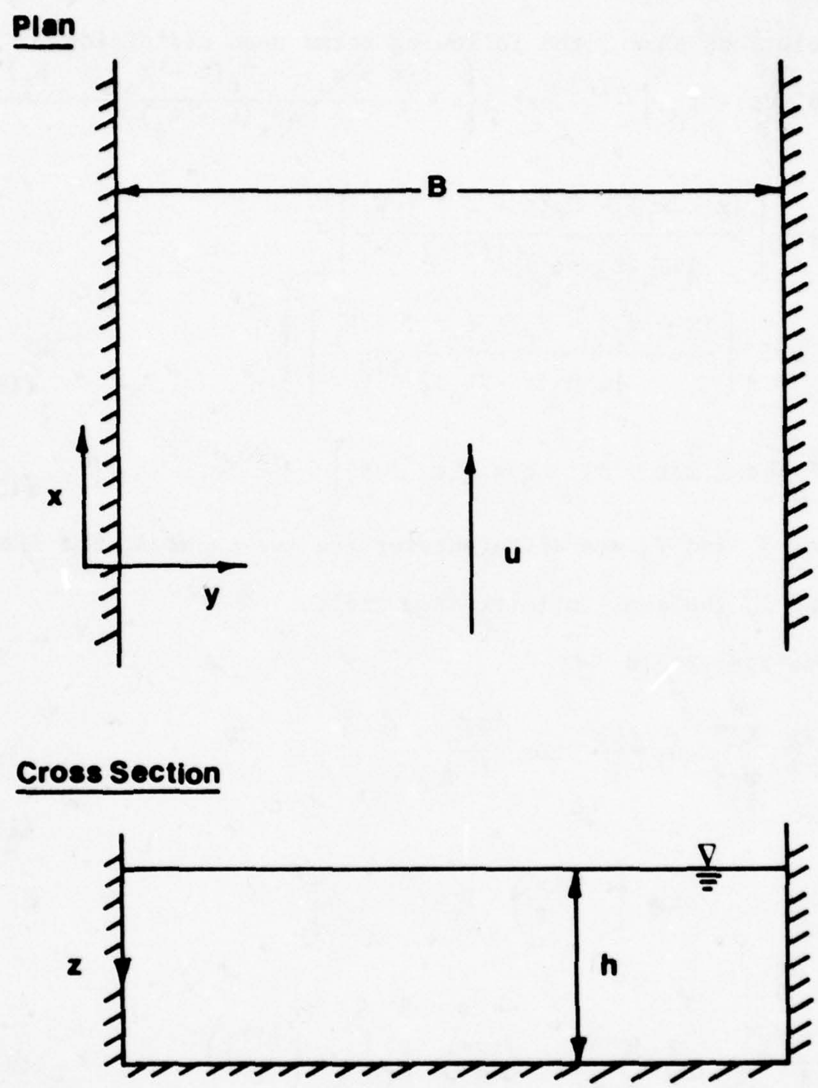

Figure 12. Coordinate System

$$\cdot X_2(x,t)Y_2(y,t)$$

$$\cdot Z_2(z,t)\ dt_o \qquad (104)$$

In the solutions shown, the following terms need definition.

$$X_1 = \left\{4\pi D_x(t - t_o)\right\}^{-1/2} \exp\left\{-\frac{\{(x - x_s) - U_f(t - t_o) + W_1\}^2}{4D_x(t - t_o)}\right\} \qquad (105)$$

$$X_2 = \frac{1}{2}\left\{\mathrm{erf}\left[\frac{(x - x_1) - U_f(t - t_o) + W_1}{\{4D_x(t - t_o)\}^{1/2}}\right] - \mathrm{erf}\left[\frac{(x - x_2) - U_f(t - t_o) + W_1}{\{4\ D_x(t - t_o)\}^{1/2}}\right]\right\} \qquad (106)$$

$$W_1 = \left(\frac{U_{max}}{\omega}\right)\left[\cos\omega(t + \delta) - \cos\omega(t_o + \delta)\right] \qquad (107)$$

Values for Y_1 and Y_2 are different for the two cases, A, the finite flow field, and B, the semi-infinite flow field.

Case A - Finite Flow Field

$$Y_1 = \frac{1}{B} + \frac{2}{B}\sum_{i=1}^{\infty} \cos\frac{i\pi y}{B}\cos\frac{i\pi y_s}{B} \cdot \exp\left[-\left(\frac{i\pi}{B}\right)^2 D_y(t - t_o)\right] \qquad (108)$$

$$Y_2 = \frac{y_2 - y_1}{B} + \frac{2}{B}\sum_{i=1} \cos\left(\frac{i\pi y}{B}\right)\frac{B}{i\pi}\left\{\sin\left(\frac{i\pi y_2}{B}\right) - \sin\left(\frac{i\pi y_1}{B}\right)\right\}\exp\left[-\left(\frac{i\pi}{B}\right)^2 D_y(t - t_o)\right] \qquad (109)$$

Case B - Semi-Infinite Flow Field

$$Y_1 = \{4\pi\ D_y(t - t_o)\}^{-1/2}\left[\exp\left\{-\frac{(y - y_s)^2}{4D_y(t - t_o)}\right\}\right. \qquad (110)$$

$$+ \exp \left\{ - \frac{(y + y_s)^2}{4\, D_y (t - t_o)} \right\} \Bigg] \Bigg]$$

$$Y_2 = \frac{1}{2} \left\{ \operatorname{erf} \left[\frac{y + y_2}{\{4\, D_y (t - t_o)\}^{1/2}} \right] - \operatorname{erf} \left[\frac{y + y_1}{\{4\, D_y (t - t_o)\}^{1/2}} \right] \right.$$

$$\left. - \operatorname{erf} \left[\frac{y - y_2}{\{4\, D_y (t - t_o)\}^{1/2}} \right] + \operatorname{erf} \left[\frac{y - y_1}{\{4\, D_y (t - t_o)\}^{1/2}} \right] \right\} \qquad (111)$$

Expressions for the remaining terms are the same for either model, A or B.

$$Z_1 = \sum_{j=1}^{\infty} \psi_j (z) \psi_j (z_s) \exp \left[-k_j^{\,2}\, D_z (t - t_o) \right] \qquad (112)$$

$$Z_2 = \sum_{j=1} \psi_j (z) \left(\frac{b_j}{k_j} \right) \left\{ \sin k_j\, z_2 - \sin k_j\, z_1 - \frac{K_e}{C_p \rho\, D_z k_j} \right.$$

$$\left. \cdot (\cos k_j z_2 - \cos k_j\, z_1) \right\} \exp \left[-k_j^{\,2}\, D_z (t - t_o) \right] \qquad (113)$$

with

$$\psi_j (z) = a_j \left\{ \cos\, (k_j z) + \frac{K_1}{D_z k_j} \sin\, (k_j z) \right\} \qquad (114)$$

k_j and a_j being given by

$$\tan (k_j h) = K_1 / D_z k_j \qquad (115)$$

and

$$a_j^{\,2} = \left\{ h \left[1 + (K_1/D_z k_j)^2 \right] + (K_1/D_z k_j) \right\}^{-1} \qquad (116)$$

An important note should be added here. If both K_1 and K_2 are zero, then a term of $1/h$ must be added to Equation (112), increasing Z_1 by $1/h$.

i. Application of Yeh and Tsai Model - Anyone who has waded through the preceding equations (or, which is more likely, has skimmed to this paragraph)

is aware that this analytical solution will require use of a computer to evaluate c (x,y,z,t). Yeh and Tsai (135) have developed a program to perform the solution for these four sources and plane and line sources oriented parallel to other axes also. It is, however, a proprietary program at present and cannot be released. Yeh (137) notes that considerable programming effort and testing had to be devoted to getting this model operational. It was believed beyond the scope of this current work to attempt this sort of programming effort. However, it might prove worthwhile in future work.

2. Coefficient Selection Problems - Yeh and Tsai (135) present results of two field studies being fit to the model and report the coefficients for those cases. It is interesting to compare those fitted values to standard values. Ultimately, of course, the ability to predict without dye data is a major goal of any such model. In order to obtain a view of the magnitude of the coefficients in the form of Eqn.(32), a few simple assumptions were made. As typical values of u/u_* range from 10-20, u_* was taken as 1/15 U_{max}, where U_{max} is the maximum tidal component of velocity. It should be noted that average values over the tidal cycle would be less than this, and hence actual values of α might be expected to be higher than those reported in Table 4. In case 1, U_{max} is 208 meters/hour (0.19 feet/second), with h = 13 meters (42 feet). In case 2, U_{max} is 610 meters/hour (0.55 feet/second), with h = 12 meters (40 feet). Case 1 is in the Hudson River, with an average width of about 945 meters. Case 2 is in Long Island Sound. Cases 1 and 2 refer simply to the two sites they studied.

The double designation of the longitudinal and transverse coefficients acknowledges the fact that the coefficients in the partially averaged-three dimensional equation are not identified to the coefficients in Equation (11). The concern here is the values for α. The vertical term is probably satisfactory and not terribly important in any event. On the other hand, values for the transverse and longitudinal coefficients are much larger than one

would probably choose if the model were to be used in a predictive mode with no data existing. The transverse coefficients may be an order of magnitude greater. There is less certainty about the longitudinal values. However, since the width-to-depth ratio at the sites is about 70 to 1, it seems likely that values for the longitudinal coefficient would be less than that due to the full lateral variation of longitudinal velocity. In any event, case 1 has an α value about equal to that for the Missouri River at one site (58).

TABLE 4. COEFFICIENTS FROM YEH-TSAI MODEL VERIFICATION

	Case 1		Case 2	
Coeff.	Value, m^2/hr (ft^2/sec)	α	Value, m^2/hr (ft^2/sec)	α
D_x (D_L)	1.1×10^6 (3290)	6200	9.3×10^5 (2780)	1880
D_y (e_y)	3700 (11)	21	14,000 (42)	28
D_z	33 (0.1)	0.186	18.6 (.06)	.04

A review of the work done by Holley, et al (82) indicates that for estuaries this wide, the D_x value due to shear only is likely to approach Elder's value of $6hu_*$ based on vertical variations only. However, Fischer's (24, 25) discussions on contributions to longitudinal mixing in the 1-D equation indicate numerous possible contributions to D_x beyond simply the shearing action. Recall that Fischer notes that in some cases the currents generated by unusual geometry (overbanks, etc.) may be the major component of the longitudinal dispersion term. These same currents could lead to the inflated transverse coefficient values.

Insufficient information is presented in Reference 135 to assess the reasons for the inflated coefficients. In this particular case, selection of

standard coefficient values would probably yield conservative estimates of concentrations, but it is possible they might be too conservative. Only by proper review of site geometry, stratification, and sensitivity testing of the model will it be possible to make more definitive statements about the values reported here. Use of this example is not intended to downgrade the model, but rather to emphasize the need for reviewing carefully the averaging which has occurred to arrive at a given equation and the physical forces at work at each site for the given discharge history. The complexity of this particular model makes it difficult to state exactly what advective behavior is lumped into the coefficients. However, a few items are worth noting.

Transverse velocities, v, are neglected, and any such currents would lead to changes in the magnitude of D_y.

Equation (93) specifies a velocity varying only with time, not with distance, x. This can be a problem if travel time to the point of interest is a significant portion of a tidal cycle. This appears to be the case in the field work reported by Yeh and Tsai (135). In *addition, width variation* in the estuary would lead to variation of u with x even if steady flow existed. Over the 1500 meter study area (in x direction) the width in case 1 (see Table 4) appears to vary from about 600 to 1200 meters. Not only does this suggest considerable variability of u with x, it also suggests the existence of a reasonable transverse velocity component, v. If the depth also varies across the channel, differential advection due to this variation would also be lost by assuming constant h. Therefore, a number of advective terms have been neglected or simplified and must then be compensated for by the coefficients. No solution currently exists quantifying the individual contributions.

WANG, ET AL TIDAL FJORD MODEL AND KUO MODEL

Another example of an analytical solution by integral transforms

is that given by Wang, et al (138), based on earlier developments by Wang, et al (139 and 140). While a number of elements are similar to the model of Yeh and Tsai (135), there are some differences which make it instructive to briefly review this model. Two solutions are presented, for an instantaneous point source and for a continuous point source. Proper integration, numerically or analytically, of these point source relationships can yield any spatial source configuration, similar to the work of Yeh and Tsai (135). However, these are not presented in their papers.

Other assumptions of interest are listed below.

Dispersion is allowed in x,y,z directions.

Only a longitudinal velocity component, u,is included, or $v=w=o$.

The velocity u is a function of z (the vertical ordinate) and t only. Its vertical variation is assumed linear, in the form of Equation (117).

$$u(z,t) = z(a - b \cos \omega t) \tag{117}$$

in which a, b are constants

It is assumed that the point source is of sufficient distance from any horizontal bounding plane (water surface, channel bottom, or interface between density-stratified fluids) so that the tracer does not reach such a boundary. Wang, et al (138) note that one example is the strait of Canso, where the depth is about 0.50 kilometers(1600 feet).

The fluid is bounded laterally, at $y = o$ and $y = B$.

A quick review shows that this is essentially the same as one subset of the Yeh-Tsai model, that for a point source with the upper and lower boundaries placed at very great distances. The only real distinction lies in the velocity, which is assumed to vary vertically, although there is some question as to the realism in a linear profile. Therefore, the Wang, et al (138) solutions look very much like Equation (101) except for the inclusion of

131

terms representing the vertical shear. It is interesting to note that the same solution would also hold if Equation (117) were representative of the lateral variation of velocity and the lateral boundaries were assumed at a large distance away. This could be accomplished by merely switching the coordinates y and z and interchanging the width, B, and depth, h. This could be representative of a portion of a flow field, perhaps in the middle of a large tidal estuary.

1. Application of Model - Wang, et al (138) report some numerical experiments they performed using the model. As obviously expected, they found that vertical shear increased the dispersion beyond that expected if the same D_x were used with no vertical velocity gradient. They did report a couple of peculiar results. For an instantaneous point source located near either channel bank, they show that for some parameter combinations they obtain not only a multiple peaked concentration vs. time curve at certain locations, but show periods of time during which the concentration suddenly drops to zero and remains so for a length of time dependent upon the magnitudes of a and b in Equation (117). They suggested that this multipeak distribution is a result of interaction between the unsteady current and the impermeable boundary. Of course, it is also possible that some of this behavior is an artifact of the model as well.

2. Coefficient Selection - No data fittings are reported, so no numerical coefficient values exist to compare against standards. In theory, the allowance for a vertical variation of velocity, to the extent that it is a realistic variation, should mean that the value of D_x chosen should be less than D_L, the longitudinal dispersion. This is because one portion of the advective behavior has been built back in. However, recall the statements on the Yeh-Tsai model about neglect of x variation of velocity. This clouds the issue. In addition, if the assumed velocity profile is not realistic, then it becomes

difficult to assess the change in the coefficient. If the assumed profile were realistic, a gross first approximation could be made by assuming the contributions to D_x were additive and subtracting out Elder's $6hu_*$ from the D_L value.

3. Comments - The Wang, et al (138) model presents one added feature, but is generally less versatile than the Yeh-Tsai (135) model. In addition, the increase in description of the advective field really does not make it any easier to choose coefficients. It still may eventually prove useful for discharges into very deep waters (at some depth below the surface), but there are limitations on intelligent use of the model now.

4. Kuo (113) Model - Kuo (113) has presented an analytical solutions. obtained by integral transform methods. It again can be viewed as a subset of the Yeh-Tsai (135) model. It deals with a point source discharging into a constant parameter river or estuary. That is, the discharge may be unsteady, but the receiving water flow parameters - u,h, diffusion coefficients, etc. - are constant. This obviously more restrictive than the Yeh-Tsai (135) sinusoidal velocity variation, Equation (93) which can reduce to a constant velocity by setting $U_{max} = o$,

Kuo's model, or the Yeh-Tsai reduction to it, might be useful in rivers for steady flow cases. In such cases, all neglected advective behavior must be accounted for in the coefficients, based on reasoning such as that discussed in Section III. If this model were applied in an estuary, then it would have many of the drawbacks of the non-tidal advective models in the coefficient values, as all the neglected time variation must be lumped into the longitudinal coefficient. Kuo (113) presents a comparison with time- and spatially - averaged dye data taken along a portion of the Potomac River. From data in the paper, the average depth, h, appears to be 16 to 18 feet, with u (the average velocity over a tidal cycle) = 0.455 miles/day, presumably primarily

due to freshwater flows. He reports the following best fit values for the coefficients D_x, D_y, and D_z (all in mi^2/day) = 2.64, 0.066, and 0.08. One interesting feature immediately is that D_z is larger than D_y, a feature not usually expected. It may be that the shallow depth may generate more turbulence due to bottom configurations, or data inadequacies might be the cause, or the averaging Kuo employed along with equation inadequacies may be partially or fully responsible. In a manner similar to the Yeh review, u_* was taken as 1/15 u to roughly evaluate α from Equation (32). Doing this yields approximate α values for the x,y, and z directions, respectively, of 26,400, 660, and 800. These are obviously way out of line with standard coefficient values, suggesting that the model neglects a lot of advective behavior which must be important in this case and, in general, indicating difficulties in using this sort of model in a completely predictive mode with no data.

IMAGE SOLUTIONS BY PRAKASH AND BENEDICT

The most comprehensive set of solutions by the method of images to data has been presented by Prakash (109). A number of systematic errors in the application of the method of images was discovered and corrected during the course of review for this report by Benedict (110). The work is intended for use in rivers and is comparable to the work by Yeh and Tsai (135) except that in the Prakash and Benedict work, the velocity is a single, constant value. Solutions are presented for spatial sources ranging from a point to a volume source discharging into a channel with a finite width (from y=o to y=B) and finite depth (z=o to z=h). The coordinate system is shown in Figure 12.

A few of the more interesting solutions will be presented here for both instantaneous and continuous discharges. The point source solutions for both cases have already been given as Equations (82)and (83). Relationships for some finite time for any of the source conditions can be obtained from the instantaneous solutions by time integration numerically, as discussed earlier.

Vertical Line Source - Instantaneous:

Location: $y=y_o$, from $z = z_1$ to $z = z_2$

$$C(x,y,z,t) = \frac{M \exp(-\lambda t)}{8\pi t(D_x D_y)^{1/2}(z_2-z_1)} \quad \exp - \frac{(x-ut-x_o)^2}{4D_x t}$$

$$\cdot \sum_{m=-\infty}^{m=+\infty} \sum_{n=-\infty}^{n=+\infty} F_1(t) \cdot F_2(t) \qquad (118)$$

in which M = total volume of spilled tracer material

$$F_1(t) = \exp\left[-\frac{(y-y_o-2nB)^2}{4D_y t}\right] + \exp\left[-\frac{(y+y_o-2nB)^2}{4D_y t}\right] \qquad (119)$$

$$F_2(t) = \mathrm{erf}\left[\frac{z+z_2-2mh}{2(D_z t)^{1/2}}\right] - \mathrm{erf}\left[\frac{z+z_1-2mh}{2(D_z t)^{1/2}}\right]$$

$$+\mathrm{erf}\left[\frac{z-z_1-2mh}{2(D_z t)^{1/2}}\right] - \mathrm{erf}\left[\frac{z-z_2-2mh}{2(D_z t)^{1/2}}\right] \qquad (120)$$

Continuous Vertical Line Source:

$$C(x,y,z) = \frac{C_o Q_o \exp(-\lambda x/u)}{4(z_2-z_1)u(\pi x D_y/u)^{1/2}} \cdot$$

$$\sum_{m=-\infty}^{m=+\infty} \sum_{n=-\infty}^{n=+\infty} F_1(x/u) \cdot F_2(x/u) \qquad (121)$$

in which $F_1(x/u)$, $F_2(x/u)$ implies use of Equations (119) and (120), respectively with x/u replacing t.

The plane source represents a source in the yz plane discharging material in the x direction. Notice in the plane source continuous solution, as in the continuous line source [(Equation (121)] that D_x is not included in the solution,

having been assumed negligible in a steady-state case.

Plane Source - Instantaneous:

Location: $z = z_1$ to $z = z_2$, $x = x_o$, $y = y_1$ to $y = y_2$

$$C(x,y,z,t) = \frac{M \exp(-\lambda t)}{8\,(y_2 - y_1)\,(z_2 - z_1)\,\sqrt{\pi D_x t}} \cdot$$

$$\exp\left[\frac{(x - ut - x_o)^2}{4 D_x t}\right] \cdot \sum_{m=-\infty}^{m=+\infty} \sum_{n=-\infty}^{n=-\infty} F_2(t) \cdot F_3(t) \tag{122}$$

in which

$$F_3(t) = \text{erf}\left\{\frac{y + y_2 - 2nB}{2(D_y t)^{1/2}}\right\} - \text{erf}\left\{\frac{y + y_1 - 2nB}{2(D_y t)^{1/2}}\right\}$$

$$+ \text{erf}\left\{\frac{y - y_1 - 2nB}{2(D_y t)^{1/2}}\right\} - \text{erf}\left\{\frac{y - y_2 - 2nB}{2(D_y t)^{1/2}}\right\} \tag{123}$$

Plane Source - Continuous:

$$C(x,y,z) = \frac{c_o Q_o}{4} \exp(-\lambda x/u) \cdot$$

$$\sum_{m=-\infty}^{m=+\infty} \sum_{n=-\infty}^{n=+\infty} F_2(x/u) \cdot F_3(x/u) \tag{124}$$

in which $F_3(x/u)$ implies use of Equation (123) substituting x/u for t.

Note that in all instantaneous releases, the variable t is the time from the release time. For numerical integration assuming a series of concentrated instantaneous releases, this t might be replaced by $(t-t_o)$, in which t_o is the time of release of a slug of material, and would differ for each assumed instantaneous release in the series.

Volume Source - Instantaneous:

Location: $x = x_1$ to x_2, $y = y_1$ to y_2, $z = z_1$ to z_2

$$C(x,y,z,t) = \frac{M \exp(-\lambda t)}{8\,(x_2 - x_1)\,(y_2 - y_1)\,(z_2 - z_1)} \cdot$$

$$\left\{ \operatorname{erf} \frac{x - ut - x_1}{2\sqrt{D_x\, t}} - \operatorname{erf} \frac{x - ut - x_2}{2\sqrt{D_x\, t}} \right\} \cdot F_2(t) \cdot F_3(t) \qquad (125)$$

The continuous volume source solution is not presented by Prakash (109), although it could be obtained by integration of Equation (125) with time, or by solution of the basic differential equation neglecting D_x. Some results by numerical integration of Equation (125) are presented in Section VI.

One way of verifying partially published equations one must evaluate is to assure that they collapse to simpler available solutions. For example, Benedict (110) notes that Equation (124) collapses to Lau's (141) two-dimensional plane source solution by setting z_1=o and z_2=h. Also, Holley, et al (18) present the solution for an infinite vertical line source [(Equation (77)]. Again, both Equations(124) and (121) collapse to that solution. Prakash's original versions did not do either of these.

Benedict (142) has discussed application of this model system. The coefficients to be chosen must include all the advective behavior discussed in Sections II and III, as only the mean velocity, u, is included. It is expected, for example, that D_x will have a value near D_L, the longitudinal dispersion coefficient, if the plume covers any reasonable portion of the cross-section. A number of numerical examples will be given using this model set in Section VI. It is much easier to get these models operational, as there are no convergence problems with the series involved.

STREAM TUBE MODEL SOLUTIONS

The stream tube approach, using a natural system of coordinates and the cumulative discharge as the independent variable, was discussed in Section II. Figure 1 illustrates the system, described by Equations (28) through (31).

Solutions to Equation (31) have been obtained in three ways, each of which will be briefly discussed here: (1) analytical solutions, (2) numerical solutions, and (3) a combination of the two in longer reaches of rivers. Recall that this is for a steady - state condition. The approach to be ultimately selected depends on the flow characteristics and the degree of accuracy required.

Yotsukura and Cobb (36) showed that solutions of Equation (31) for $m_x = 1$ are not too sensitive to variations in the specific distribution of $h^2 u_x D_y$ with respect to q_c, as long as its averaged value over the total river flow, Q, remains the same. This finding coupled with their further experience indicates that one can, for many natural channels, obtain a reasonable approximation by defining a constant diffusion factor as

$$D_f = m_x h^2 u_x D_z \tag{126}$$

with this definition, Equation (31) can be rewritten in a very simple form, as

$$\frac{\partial c}{\partial x} = D_f \frac{\partial^2 C}{\partial q_c^2} \tag{127}$$

Solutions to this one-dimensional Fickian model are readily available for many boundary conditions. Yotsukura and Cobb (36) give the following dimensionless solution for a point source discharging continuously.

Point Source at $x = o$ and $q_c = q_s$:

$$C'(\alpha, q') = \frac{A_1}{(2\pi)^{1/2}} \sum_{n=o}^{\infty} \left\{ \exp\left[-\frac{A_1^2}{2}(2n+q_s' - q')^2\right] + \exp\left[-\frac{A_1^2}{2}(2n + q_s' + q')^2\right] \right\}$$
$$+ \sum_{n=1}^{\infty} \left\{ \exp\left[-\frac{A_1^2}{2}(2n - q_s' - q')^2\right] + \exp\left[-\frac{A_1^2}{2}(2n - q_s' + q')^2\right] \right\} \tag{128}$$

in which

$$c' = \frac{c}{\bar{c}} \tag{129}$$

$$\bar{c} = \text{avg. concentration} = \frac{1}{Q} \int_0^Q c\,dq \tag{130}$$

$$q' = \frac{q}{Q} \tag{131}$$

$$q_s' = \frac{q_s}{Q} \tag{132}$$

$$A_1^{\,2} = \frac{Q^2}{2D_f x} \tag{133}$$

Notice the similarity of this solution form to the earlier image solutions for C(x,y,z). As expected, any spatial source conditions can be simulated by the superposition principle. Yotsukura and Cobb (36) define the solution for a line source extending from q_{s1}' to q_{s2}' . This means it is a line source extending laterally across the river from the point where the cumulative discharge is q_{s1}' to the point where it is q_{s2}'. Recall that this model gives depth-averaged concentration values, and hence a line source here is actually a plane source covering the entire river depth. The solution for this distributed source can be written as (36).

Plane Source - Stream Tube Model:

$$C'(\alpha,q') = \frac{1}{2(q_{s2}' - q_{s1}')} \left[\sum_{n=o}^{\infty} \left\{ \operatorname{erf}\frac{A_1(q_{s2}' + 2n - q')}{\sqrt{2}} - \operatorname{erf}\frac{A_1(q_{s1}' + 2n - q')}{\sqrt{2}} + \operatorname{erf}\frac{A_1(q_{s2}' + 2n + q')}{\sqrt{2}} - \operatorname{erf}\frac{A_1(q_{s1}' + 2n + q')}{\sqrt{2}} \right\} + \sum_{n=1}^{\infty} \left\{ \operatorname{erf}\frac{A_1(q_{s2}' - 2n - q')}{\sqrt{2}} \right. \right.$$

$$- \operatorname{erf} \frac{A_1 (q_{s1}' - 2n - q')}{\sqrt{2}} + \operatorname{erf} \frac{A_1 (q_{s2}' - 2n + q')}{\sqrt{2}}$$

$$\left. \left. - \operatorname{erf} \frac{A_1 (q_{s1}' - 2n + q')}{\sqrt{2}} \right\} \right] \qquad (134)$$

The Nuclear Regulatory Commission (NRC) has published solutions similar to those by Yotsukura and Cobb (36) but has the solution obtained by integral transform methods (143).

1. Particular Applications and Diffusion Factor - Yotsukura and Cobb (36) and Yotsukura and Sayre (38) give examples showing that data plotted against cumulative discharge, q_c, rather than lateral coordinate, y, conform much more closely to a Gaussian lateral profile. A number of interesting advances and applications have been made using the stated solutions or modified versions of them. Most of this work has been guided by Yotsukura with the United States Geological Survey (USGS) and by Sayre at the University of Iowa. Yotsukura and Sayre (38) review a number of these works. More have surfaced since that time. Jackman and Yotsukura (131) have extended earlier work reported by Yotsukura (37) and Jobson and Yotsukura (144) describing the thermal regimes of rivers thermally loaded by power plants and other large cooling water users. This procedure involved a patching together of solutions to Equation (127) with exponential attenuation of temperature due to atmospheric exchange as it travels downstream. It has proven highly successful in rivers such as the Potomac, yielding accuracies within about 1°C when compared with field data.

Sayre and Caro - Cordero (22), Caro - Cordero and Sayre (145), and Paily and Sayre (146) all report on the use of the stream tube model to simulate the behavior of shore-attached thermal plumes, which also are essentially mixed to the stream bottom. A variety of means are used to estimate the initial dilution the discharge undergoes when it is bent up against the shoreline

by the ambient velocities frequently exceeding initial heated water discharge velocities. Once this initial dilution is estimated or determined from data, an estimate of total flow in the plume (initial heated discharge plus ambient river water entrained into the plume) can be made. This flow can be assumed to be that portion of the total river flow occupied by the plume and thus give the size of the initial plane source for the diffusion solution. In addition, the estimated dilution yields the assumed initial concentration at the location of that plane source. Probably the most satisfactory way to handle this problem is to use one of the available jet models for initial mixing if applicable. Unfortunately, the cases in the Missouri are not amenable to treatment by the standard models. However, in situations where the initial discharge velocity is greater than the ambient velocity, it might be possible to use this approach. In the work described by Sayre and Caro - Cordero (22), the plane source is attached to the bank; in cases where a more definite initial jet behavior exists, the plane source might be located at some distance from the shore.

2. Numerical Models - Numerical solutions to Equation (127) are preferable in situations where greater accuracy is required and sufficient data about channel geometry and D_y variation is available to assure that this accuracy can be achieved. Yotsukura and Sayre (38) briefly describe a simple explicit forward difference finite difference scheme which has been used by Chang (13), Sayre and Yeh (40), and, in the form often called Fischer's routing method in the literature by Yotsukura, et al (54). This method has been well documented and successfully used for a number of steady-state studies. Note the important fact that unless good data on geometry and diffusion rates exist, then no increase in accuracy can be expected by use of the numerical models, and an analytical solution makes much more sense. In addition, many times, the analytical solution provides all the information that can be used.

3. Combined Analytical and Numerical Approach - Yotsukura (37) and Jobson and Yotsukura (144) report on a combined approach for simulation of large-scale river systems with confluences, bends, and islands. The method has been documented and a computer program available (132), but more work appears needed on it. The system is broken up into a series of subreaches (determined mainly by location of tributaries, sharp bends, sources, rapid changes in channel geometry, etc.) and subchannels where branched flow exists. The superposition principle is used to generate concentrations at the downstream end of each subreach or subchannel from known transverse distributions at the upstream end. These new values then become the known condition at the head of the next subreach downstream. This method also requires good knowledge of channel geometry and diffusion characteristics.

4. Diffusion Factor - The lumped diffusion factor, D_F, is a term including many effects. The most comprehensive review of its variation has been presented by Caro - Cordero and Sayre (145) and Sayre and Caro - Cordero (22). Recall that if the average value of the diffusion factor is the same, the exact distribution is not critical for many cases. The average value is defined from

$$Q^2 D_f = \int_0^1 m_x h^2 u D_y \, dq' \tag{135}$$

Recall that in all these uses, the various parameters -u, D_y, etc. - are depth averages. Using the assumption that D_y is constant across the river, and a semi-empirical relationship presented by Yotsukura and Sayre (36) based on earlier Missouri River dye studies, the following relationship can be developed (22):

$$BD_f = 0.4 \left(\frac{P_1}{\bar{h}^2 \bar{u}}\right)\left(\frac{B}{\bar{h}}\right)\left(\frac{\bar{u}}{u_*}\right)\left(\frac{\bar{h}}{R_c}\right)^2 \tag{136}$$

in which $\bar{h}$ = average depth over cross-section

$\bar{u}$ = average velocity over cross-section

R_c = radius of curvature of bend

$$P_1 = \int_0^1 m_x h^2 u dq'$$

Additional data by Caro-Cordero and Sayre (145) also seemed to fit Equation (135) reasonably well, although some scatter does exist. When laboratory data are compared with Equation (136), however, they generally show much higher (7-8 times) the value of D_f for the same value of the right-hand side of Equation (136). The writers reporting these findings note that the reason for such differences is unknown. It will be beneficial in the future to compare the findings reported by Krishnappan and Lau (19) in a laboratory flume and discussed in Section III under bends. Note they got lower values for D_y than Chang (13), possibly due to the more realistic cross-section shape. It may be that the uniform cross section in some lab studies may be a part of the cause of the discrepancy. In any event, Equation (136) does provide a beginning point. Further work will resolve some of the current uncertainties.

NON-TIDAL ADVECTIVE MODELS

Section II discusses time averaging over longer times, such as tidal cycles, and one-dimensional Equations (26) and (27) are presented. In both of these one-dimensional equations all the advective behavior is contained in the fresh water flow term and tidal action is neglected. Hence, the longitudinal coefficient D_L (or $\bar{D}_L$ or D_{Ls}) must attempt to account for any longitudinal mixing due to tidal motion. Recall that the different coefficient designations result from the three separate averaging processes employed.

There are a number of reasons why these non-tidal models may not be as useful as they were several years ago. First, several questions have been

raised about the validity of 1-D equations in many systems. Second, a number of good, real-time 1-D numerical models exist which incorporate all the advective properties (134, 75, 78) and decrease the need for difficult evaluations of D_{Ls} or $\bar{D}_L$. Third, models such as those by Yeh and Tsai (135) are appearing which represent analytical solutions including a time-varying velocity. Difficulties of coefficient selection as discussed under that model may put it into somewhat the same category as the non-tidal models, but it should have greater long-term utility. Fourth, if a spill or short-duration discharge occurs, the time scale of this release may be much smaller than the averaging time of the tidal period ($\bar{D}_L$) or time between slack water (D_{Ls}) and therefore make meaningless any prediction of effluent behavior based on such average conditions. This is an especially telling restriction in the case of accidential spills, especially when several days may be required for a discharge to continue in order to attain some equilibrium within a tidal water body. Quite obviously, the behavior of a finite-duration spill at any given site is very strongly a function of what portion of the tidal cycle the discharge covered. This can not in any way be reflected by the non-tidal models. Their use in such cases should be avoided.

Despite the rather severe shortcomings of these models for general use in spill analysis, they do have some advantages, such as:

• There is a substantial body of literature on these models, and they have often been used or recommended by various regulatory agencies (147).

• If discharge duration is fairly long, the models can provide, with judgement, a first estimate of a given situation.

• Substantial experience, including dye studies, exist with these models. If a discharge occurs into one of the water bodies where coefficients have previously been estimated based on data, a higher order of confidence can be assigned to predictions there. This is especially true in cases where it is

difficult to evaluate coefficients needed for some alternative model.

- Some possibility exists for use of numerical models to calibrate these non-tidal models. Numerical output is fitted to the non-tidal model as some kind of numerical dye data. The dispersion coefficients determined by this fitting extends use of the non-tidal models over a wider range of conditions.

Note that none of these points overcome the inadequacy for short duration spills, because the spill may be much shorter than the tidal period averaging time. This long averaging time neglects the substantial difference in mixing characteristics at different times in the tidal cycle.

In addition to original References (30 & 31), there are a number of places where discussions of one or more solutions to Equation (26) or (27) appear, including O'Connor and Thomann (148), NRC (143), Thomann (149), among others. Since the case is 1-D, the source is always assumed distributed completely across the section. The primary building block is the instantaneous, or impluse, release. Finite duration solutions can then be obtained by time integration.

1. Instantaneous Release - The first case considered is that of an instantaneous source discharged such that the material is assumed uniformly distributed over the cross-section at x = o. A mass M is released over the cross-sectional area A.

$$C(x,t) = \frac{M}{2A\sqrt{\pi D_{Ls} t}} \exp\left[\frac{-(x-U_f t)^2}{4D_{Ls} t} - \lambda t\right] \qquad (137)$$

The designator D_{Ls} is used instead of D_L assuming that this is the solution to the slack tide approximation, Equation (27). Virtually everything that will be said in the next several paragraphs could also apply to Equation (26) for averages over a tidal cycle, but the slack tide designation will be used

here. Equation (137) yields a Gaussian curve when viewing the x variation at a given t. If the variation with t at a given x is reviewed, the distribution is a symmetrical, with the degree of skewness dependent upon the relative magnitude of the terms $U_f t$ and $(4D_L t)^{1/2}$. The skewness takes the form of a steeper rise than Gaussian initially and a longer, slower falling tail. The use of Equation (137) through superposition, should enable formulation of any source condition.

2. Continuous Release - A continuous release can be simulated by integration of Equation (137) over time. Consider a square pluse (i.e., a discharge at a constant rate with time for a finite time, t_d, then dropping back to zero). The solution is:

$$C(x,t) = \frac{Q_o C_o}{2A\Omega} \exp\left(\frac{U_f x}{2D_{Ls}}\right) g(x,t) \quad \text{for } o<t<t_D \tag{138}$$

$$C(x,t) = \frac{Q_o C_o}{2A\Omega} \exp\left(\frac{U_f x}{2D_{Ls}}\right) \quad g(x,t)-g(x,t-t_D) \quad \text{for } t>t_D \tag{139}$$

in which

$$\Omega=\sqrt{U_f^{\,2}+4\lambda D_{Ls}} \tag{140}$$

$$g(x,t) = \left[\operatorname{erf}\left\{\frac{x+\Omega t}{(4D_{Ls}t)^{1/2}}\right\} \pm 1\right] \exp\left(-\frac{\Omega x}{2D_{Ls}}\right)$$
$$-\left[\operatorname{erf}\left\{\frac{x-\Omega t}{(4D_{Ls}t)^{1/2}}\right\} \pm 1\right] \exp\left(-\frac{\Omega x}{2D_{Ls}}\right) \tag{141}$$

In the brackets in Equation (141), the sign within the brackets is taken as negative for downstream (x positive) and positive upstream of the source (x negative). The function $g(x,t-t_D)$ is the same expression as Equation (141) with $t-t_D$ replacing t. If the pulse duration t_D continues for a very long

time, Equation (138) then represents the steady-state solution for a continuous source when large t is substituted into the equation. The equation yields very simple forms if the substance is conservative (λ=o) or if any of the terms such as U_f or D_{Ls} are assumed small. It is instructive to look briefly at these reduced forms, for they relate to things with which most readers can readily associate.

If U_f=o, upstream and downstream distributions will be symmetrical about the release point, with

$$C = \frac{Q_o c_o}{A\ (+4\lambda D_{Ls})^{1/2}} \exp\left(\sqrt{\frac{\lambda}{D_{Ls}}}\, x\right) \tag{142}$$

The key feature here is that only decay and dispersion modify the longitudinal variation, with no advection. When this form is viewed, it becomes even more evident that the coefficient D_{Ls} incorporates tidal advective characteristics into it. If dispersion were small, and U_f was not zero, then the equation for c merely becomes a first-order exponential decay equation frequently used in rivers for BOD, heat, etc., and given as

$$c = \frac{Q_o c_o}{Q} \exp\left(-\lambda x/u\right) \tag{143}$$

The key feature of Equation (143) is the illustration of the possible importance of λ. If the decay coefficient is important, it may dominate behavior. Harleman (27) gives an example for a steady-state case including tidal advective velocities where the downstream concentration is obviously dominated by decay, much as indicated by Equation (143), while tidal advection and dispersion dominate upstream conditions.

3. Holley and Harleman Real Time Solutions - Holley and Harleman (81) present real-time solutions for 1-D and 2-D cases in a uniform area estuary. It is interesting to compare their solutions with the non-tidal models. Velocity is assumed a function of time only, not of x. The longitudinal

dispersion coefficient D_L is assumed constant. The velocity is chosen as

$$u(t) = U_f + U_T \sin \sigma(t-\delta) \tag{144}$$

which is similar to Equation (93). The term δ is the phase (time) shift between the zero tidal component of velocity and the release time. The constant area estuary is assumed to have width B. Only the instantaneous release equations will be presented here, as any other discharge history can be formulated by numerical integration.

1-D Instantaneous Release:

$$C(x,t) = \frac{M \exp(-\lambda t)}{A(4\pi D_L t)^{1/2}} \exp\left(-\frac{W_2^{\,2}}{4D_L t}\right) \tag{145}$$

in which $W_2 = x - U_f t + \frac{U_T}{\sigma}\left[\cos \sigma(t-\delta) - \cos\sigma\delta\right]$

For the case of a release of mass M at t=o, x=o, at the side y=o, the following 2-D relationship is obtained.

2-D Instantaneous Release:

$$C(x,y,t) = \frac{M \exp(-\lambda t)}{2\pi h\sqrt{D_x D_y t}} \cdot \exp\left(\frac{-W_2^{\,2}}{4D_x t}\right)$$

$$\cdot \sum_{n=-\infty}^{+\infty} \exp\left(-\frac{(y-2nB)^2}{4D_y t}\right) \tag{146}$$

It should be noted that these models have similar form to the Yeh-Tsai (135) equations, which should yield the same results. The two equations reveal some interesting features. The first is seen in Equation (146). Recall earlier comments indicating that the time for cross-sectional mixing to be accomplished is on the order of $(0.4 - 0.5)B^2/D_y$. This time is such that at least two phenomena may possibly occur to prevent the system from ever behaving

as 1-D. First, the material may be flushed from the estuary by progressive spreading and advection before transverse mixing is completed. Second, if the decay is sufficient, the material may have been dissipated by this internal reaction prior to achieving 1-D conditions. Equation (146) could provide a basis for estimation of the likely applicability of a 1-D model to a given case. Note that D_x to be used in Equation (146) is probably on the order of Elder's $6hu_*$ inasmuch as the equation represents depth averaging. If the 1-D state is approached, however, lateral variations in velocity would mean D_x should be much larger. In general, in fact, if u is not a function of y in the equation, the larger the width covered by the plume, the larger value which must be assigned to D_x.

The one-dimensional Equation (145) can be compared with Equation (137). It can be seen to be identical except for the tidal component of the velocity. This is a critical difference, for it greatly changes the meaning of the longitudinal coefficient (D_L versus D_{Ls}). The value of D_{Ls} must be much greater to include tidal effects.

Harleman (27) presents an interesting comparison of the real time solution for a continuous discharge with the non-tidal advective solution. A quasi-steady-state solution is attained by continuing the solution to the point in time where the concentration profile along the estuary is replicated at corresponding times in each tidal cycle. For example, though it varies throughout the cycle, it would yield the same distribution at each low water slack. The following case was considered.

Comparison Case Data:

$U_f = 0.1$ feet/second

$U_T = 2.0$ feet/second

T = 44,712 seconds (12.4 hours)

$D_L = 65$ ft^2/sec (based on Equation (46) with n = 0.028)

$\lambda = 0.034/\text{day}$

Results of this comparison are shown in Figure 13. The slack tide approximation indicates essentially no concentration upstream of the discharge point. In fact, at x = 3000 feet, c/c_o by the slack tide equation is 0.01, and is thus too small to plot on Figure 13. Notice that the real time solution predicts concentrations up to about 30,000 feet upstream. In the downstream direction, it is apparent that the reaction rate, defined by λ, controls, and the slack tide approximation falls in between the high and low water slack predictions by the real time model.

The other curve on Figure 13 is the result of using an inflated value for $D_{Ls} = 2250\ ft^2/sec$, or about 35 times the D_L value. The shape of the concentration distribution can be seen to be quite different, and this and other attempts reported by Harleman (27) make it clear that no single value of D_{Ls} will bring the two models into agreement. Therefore, although D_{Ls} can compensate for some of the neglected advection, it can never account for all of it.

4. Summary on Non-Tidal Models - It has been the intention of this subsection to illustrate the inadequacies of non-tidal models for handling short term spills. The problems shown in Figure 13 for a continuous discharge will be magnified significantly for the case of a short term discharge. As noted earlier, existing data or experience in a particular estuary may justify use of a non-tidal model for a first estimate, but even then it should be employed with care and the results interpreted in the light of model shortcomings.

HOLLY NUMERICAL MODEL

Holly's (115) model is reviewed here briefly because it is felt that it represents a good step in the right direction if a numerical model is deemed necessary. It does not include sources and sinks, but future work could develop those. Holly solves the depth-averaged diffusion equation in a stream tube

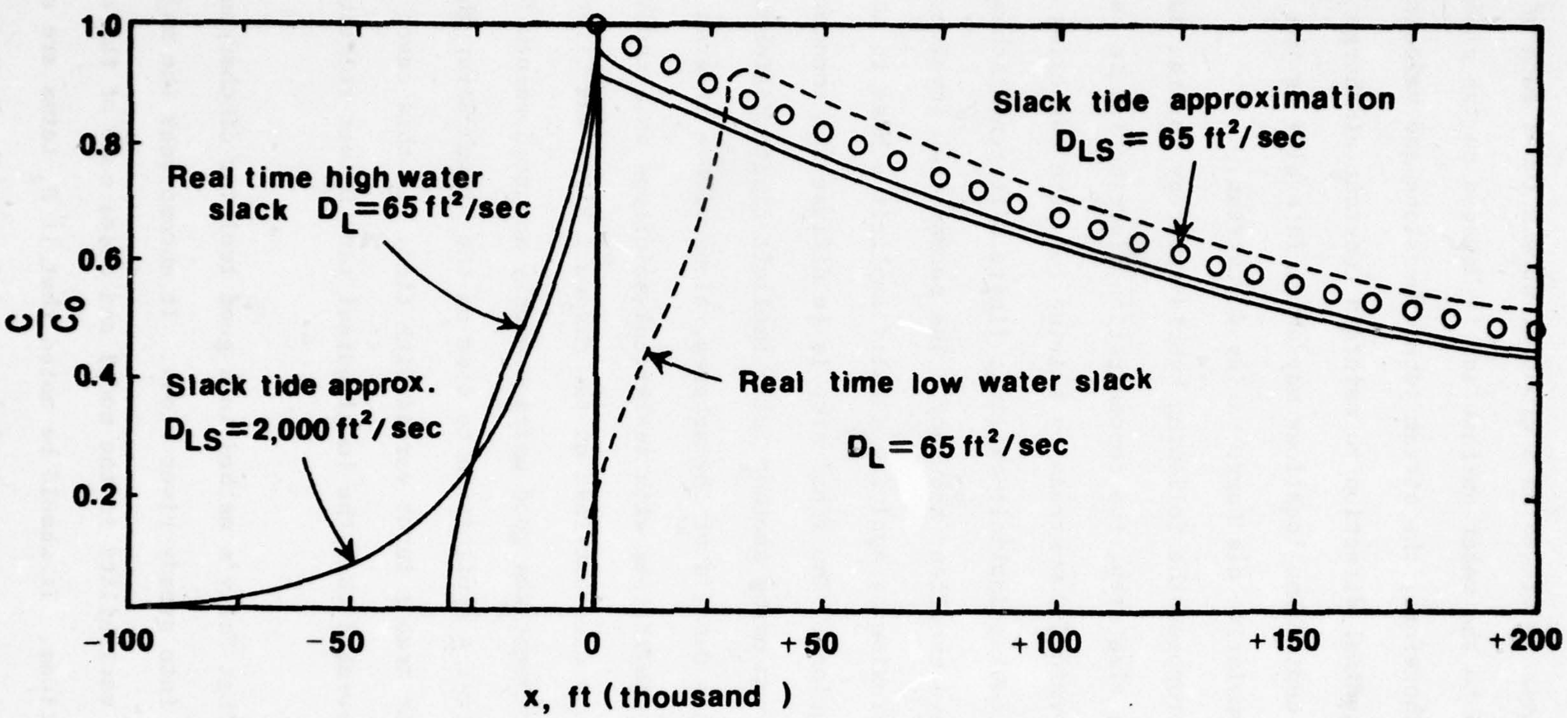

Figure 13. Comparison of Real-Time and Non-Tidal Advective Models [After Harleman (27)]

framework. The river is viewed as a group of stream tubes each of which extends from the bed to the water surface and is bounded on the sides by groups of streamlines. Therefore, the stream tube dimensions and velocities will vary in the longitudinal direction to maintain constant discharge in each. Also, stream tube centerline locations may shift laterally as the transverse distribution of cumulative discharge varies downstream.

Holly (115) proposes the following hybrid strategy for the numerical solution. In each time step, the concentration distribution in each stream tube is first determined downstream by solving for pure advection using a second order double-step implicit-explicit finite difference scheme he has demonstrated to have excellent accuracy. The second step involves solving for transverse diffusion by applying a fully implicit scheme to the previously advected concentrations. The final step is to diffuse the concentration distributions downstream using another fully implicit finite difference scheme. Holly (115) presents details of the schemes, along with a program listing. He compares model predictions with analytical solutions as a check and then applied the model to data obtained on the Missouri River and Clinch River. In both cases, agreement was good using commonly accepted values for D_x (Elder's) and D_y. He illustrates application to case on the Clinch River where river flow was steady but tracer input varied with time. In this case, numerical experimentation revealed that the longitudinal term D_x was relatively unimportant.

It is clear that Holly's method is a good tool for discharges of conservative substances into steady river flows. It encompasses the major elements of river geometry variability in the model and eases some of the concerns of coefficient selections. It should be noted that if D_x terms are actually negligible in a given case, then Holly's model looks like Equation (127) (Yotsukura's stream tube approach) for steady releases. This may mean that results

from analytical solutions for those cases would be equally as good if the river were segmented into subreaches.

The biggest single shortcoming in Holly's work for use with a spill is the lack of any source and sink terms. The hybrid finite difference scheme he has used makes it difficult to ascertain precisely where and how to include such terms in the numerical solution. It is clear it could be done, but it would be complex. In addition, testing of the numerical scheme with respect to accuracy in its handling of these additional terms would be required. There is reason to believe that this model's capabilities are sufficient to warrant this type of effort.

The model is restricted to steady receiving flows, and hence it is not applicable to tidal waters or strongly unsteady river flows. The assumption of full vertical mixing may be invalid for some distance near the source. This is no problem in shallow streams, but it might be more of a problem in deeper rivers. In those cases some sort of 3-D solution would be needed to bring the calculations to the point where the depth-averaged numerical model was applicable. A proper coupling of the two solutions would enhance the model.

In short, Holly (115) has presented a useful model of transverse mixing in steady river flows which incorporates arbitrary channel geometry. Its extension to include sources and sinks and varying source conditions could provide a valuable tool for use where the accuracy is needed.

MODELS FOR DIFFUSION IN SHEAR FLOWS

Discussion has emphasized difficulties with assuming average velocity and depth values over a section. The cumulative discharge models (stream tube models) by Yotsukura and Cobb (36) and Holly (115), for example, were considered advantageous because of the ability to incorporate realistic lateral

variations of longitudinal velocity into the solutions. Some analytical solutions including nonuniformities within the section have appeared and will be reviewed here. These models are potentially helpful in two ways. First, they are instructive in helping to understand diffusion phenomena and the relative role of diffusion and advection. Second, they may provide an ability in some water bodies to make preliminary assessments of possible effects of errors in velocity and diffusion assumptions. Recall that a key element in a realistic inclusion of the velocity field is that it makes selection of proper coefficient values easier.

1. Point Source in Uniform Shear Flow - Carter and Okubo (150) allowed the velocity in an unbounded fluid to vary linearly in both transverse and vertical directions, so that the velocity, u, in Equation (18) is written as

$$u = U + \Gamma_y y + \Gamma_z z \tag{147}$$

in which Γ_y, Γ_z are vertical, transverse gradients of velocity, respectively, with dimensions (L/T)/L Carter and Okubo (150) further assumed v=w=o and constant diffusion coefficients. For the case of an instantaneous release of tracer volume V_o with concentration C_o at (x,y,z) = (o,o,o), they obtained the following solution.

$$C(x,y,z,t) = \frac{c_o V_o}{8\pi t(\pi t \; D_x \; D_y \; D_z)^{1/2} \; (1 + \phi^2 t^2)^{1/2}}$$

$$\cdot \exp\left[- \frac{\{x - Ut - 1/2(\Gamma_y y + \Gamma_z z)t\}^2}{4D_x t \; (1 + \phi^2 t^2)} - \frac{y^2}{4D_y t} - \frac{z^2}{4D_z t} \right] \tag{148}$$

in which

$$\phi^2 = 1/12 \left[\frac{\Gamma_y^{\ 2}\ D_y}{D_x} + \frac{\Gamma_z^{\ 2}\ D_z}{D_x} \right] \tag{149}$$

Obviously, if the velocity gradients become zero, Equation (148) reverts back to the form given by Equation (79) as it should.

Okubo and Karweit (151) numerically integrate Equation (148) to achieve a continuous source. They also discuss differences in plume behavior due to the velocity gradient. Close to the source, the shear has little effect. As the plume moves downstream, the shear begins to have an effect, causing the concentration distribution to be skewed. That is, rather than a symmetrical distribution with its peak at the same y as the source, the peak will be shifted to the side of higher velocity. This occurs because less lateral mixing is able to take place in the faster velocity regions due to shorter travel times from the source.

2. Instantaneous Vertical Line Source - Monin and Yaglom (105) treated a vertical line source with u varying only with y, and D_x neglected. The velocity is defined as Equation (147), except that Γ_z = o and $U = U_o$ = the velocity at y = o. The field is unbounded laterally and of depth h. This yields

$$C(x,y,t) = \frac{c_o V_o}{4\pi h (1 + \phi^2 t^2)^{1/2}\ (D_z D_y)^{1/2}}$$

$$\cdot \exp \left[- \frac{(x - U_o t - \Gamma_y y t)^2}{4 D_x t (1 + \phi^2 t^2)} - \frac{y^2}{4 D_y t} \right] \tag{150}$$

in which ϕ is defined in Equation (149), with Γ_z = o.

In Equation (150), the value for D_x should be closer to Elder's value of

$6hu_*$ if the linear profile is reasonable over the plume area, as lateral variations are included in the velocity expression. In Equation (148), if realistic profile gradients could be specified, the value of D_x might be more like the value of turbulent diffusion longitudinally, or about $0.07hu_*$.

3. **Bounded Flow Field Solutions** - Yeh (152, 153) and Yeh and Tsai (154) have modified these earlier works by attempting to remove the restrictions of an unbounded fluid. Both models are for steady flows. Yeh and Tsai (154) present two 3-D models, one for finite width and depth (as in rivers) and the other for finite depth, infinite width (as in large lakes). Power law expressions are chosen to allow both u and D_y (and D_z in the 3-D model) to vary in the vertical direction only. This may be more realistic profile than the linear profiles mentioned in the previously mentioned studies. Work is needed, though, to provide proper parameters for the power laws for various natural cases. In addition, in many natural bodies of water, the lateral variation may be of much greater significance.

Yeh (152) and Yeh and Tsai (154) present example solutions to illustrate effects of the vertical non-uniformities. The solutions will not be reproduced here, as it is difficult to see the impact of shear in the equations directly. Yeh and Tsai (154) note that as boundary reflections start to be felt, the differences due to non-homogeneities in velocity and diffusion coefficients are cancelled out. They then conclude that these non-uniformities are only important prior to the point where boundary influences become important.

4. **Summary on Shear Flow Models** - These models are not as advanced as the other analytical models for uniform velocity fields. However, they clearly illustrate important characteristics of the interrelationship of diffusion and advection. For example, they illustrate a tendency for the plume to become

asymmetrical even if significant transverse velocities do not exist. It is reasonable to believe that some of the unbounded models might be applied for lakes or large embayments if the source is located sufficiently far from shore. Current ability to specify the velocity profile in such a system is limited, but some of the work reviewed does provide an ability to make a first-cut assessment of the sensitivity of one's predictions to assumed profiles. In fact, it might be easier to do this occasionally than to make a defensible extimate of D_x based on using a single, constant value of u.

MIT 1-D NUMERICAL MODEL

It would not be appropriate to omit discussion of a very well-conceived 1-D model developed and improved over some time by Harleman and coworkers at MIT. While this report raises serious questions about the use of 1-D models for spills in all but the smallest streams, it is still possible that this model might have some utility, either for small streams or by some sort of linkage with a model for the non- 1-D behavior.

The model now uses finite element techniques for solution of the coupled set of hydrodynamic equations (conservation of mass of water and equation of motion) with one-dimensional dispersion equations describing the behavior of any constituents of interest. The basic model is presented by Dailey and Harleman (78), who include BOD and dissolved oxygen, as well as salinity and temperature. The work by Thatcher and Harleman (75) verified the model for use in salinity intrusion regions. Brocard and Harleman (77) used it in a controlled section of river, Conowingo Reservoir, to predict temperatures, and it has been further developed to include the reactions and feedback associated with the various nitrogen forms (134). In terms of sources and sinks, it is therefore much more developed than the models reviewed herein which have included at most a first-order sink term of the form $-\lambda c$. The MIT model,

being a finite element model, can of course handle any number of sources and any time history of discharge.

The hydrodynamic model has been verified well, implying that longitudinal advection is well handled. Note that most of the verification is against water surface elevation data. The ability to reproduce this data well does not necessarily mean that all the processes contributing to longitudinal mixing are necessarily well modeled. Obviously, any processes contributing to transverse mixing are not modeled at all. The work by Thatcher and Harleman (75), resulting in Equation (57) for the longitudinal dispersion coefficient in salinity intrusion regions, also incorporated some effects of longitudinal density gradients into the equation of motion.

This model requires considerable input on geometry, flow conditions, waste loadings, and the like. However, being a 1-D model, not as much detail is required as in those by Leendertse, for example, as average values over a reach are used. However, in cases where prior assessment indicates that a 1-D model is acceptable, and where accuracy is required, this model would be a good choice. In cases with strongly 2-D or 3-D behavior of the plume, however, or where sufficient accuracy can be achieved by analytical models (at considerably less cost in time and money) other models would be preferred.

GENERAL SUMMARY ON AVAILABLE MODELS

The preceding model discussions are not intended to cover all available models, but rather to cover the types of models which are available. Others with good features will probably be appearing soon, although it is clear that no single model reviewed has all the features needed for describing general spill behavior. It would be well to review the list of needed model features given on the first page of the section. Discussions in this section have shown that one other feature is also important in some cases as a subset of item number 7. That is the ability to include varying depth and velocity

variations within the cross-section, especially in the lateral direction.

A summary of the models discussed with respect to their ability to adequately handle these requirements will be presented. However, there are some general comments which need to be made, not only to guide review of these models but also of any others which appear.

1. **Dimensionality of Equations** - The use of terms such as 3-D, 2-D, and 1-D, are very confusing in many ways. Generally, it has been used to imply diffusion or dispersion in three, two or one dimension. A glance back at just the models reviewed here shows a lot of difference in meanings of these terms when used by various authors. This sometimes can be misleading to potential users. Probably the only remedy is to carefully read all the assumptions and look closely at all the governing equations and boundary conditions. For example, several of the models are called 3-D but yet have no transverse velocities included. Section III points out clearly the importance of these velocities. In addition, the Yeh and Tsai (135) and Kuo (113) models are both called 3-D, but the former uses a sinusoidal velocity (Equation (93) while the latter is restricted to a constant velocity. Therefore, the required coefficient values and model behavior are quite different.

The message is simply to not read into the designation of dimensionality more than is really there. Check the model formulation carefully.

2. Unsteadiness - There are two sources of unsteadiness of concern. First is the unsteadiness of the source output. Second is the unsteady character of the receiving water flows. The former has been discussed frequently from the standpoint of time integration. The completely general behavior of unsteady flows in the receiving waters can currently only be accomplished in numerical models. Those analytical models incorporating receiving water flow unsteadiness (135, 81, 138) have all incorporated sinusoidal variation similar

to Equation (93). This time variation is probably reasonable in estuaries, but the behavior in rivers and reservoirs is quite different and may not be adequately represented by any simple function. It is clear that the time of release in a tidal flow is very important. No work has, however, defined the degree of river unsteadiness, if any, necessary to create a worse condition for diffusion than in a steady flow. Flow reversals can occur in areas of controlled rivers between two dams, creating complex phenomena which may not be adequately described by steady state models.

It is obvious that the whole subject of flow unsteadiness needs more attention, especially where flow reversals can occur. Criteria need to be established for use of steady-state models in these cases.

3. **Source and Sink Terms** - It is clear that it is important to be able to include conveniently all important reactions or other physical, chemical, or biological behavior which influences a given spilled material other than diffusion and advection. Such sources and sinks may include radioactive decay, uptake by chemical or biological processes (as in dissolved oxygen), settling out of material, internal absorption of heat, heat exchange across the air-water interface, or others. While solutions exist in the literature for the coupled DO-BOD reaction in 1-D cases, the analytical models noted here do not include such coupling with other constituents. It is believed that this general capability should be available in modeling the effects of spills of any toxic material. For example, a spill of hydrazine or some other material may result in excessive depletion of oxygen in the river. Even if the material were not toxic per se, if it exerted a high oxygen demand, this effect must be predicted. While the general form of the Yeh-Tsai (135) formulation includes the potential for inclusion of DO and BOD [through Equations (91) and (92)], the solution is not obtained for this case. In addition, some toxic substances

exert a very sudden, large oxygen demand followed by a more gradual use. The ability to include such behavior, if it exists for material of interest to the Air Force, is essential.

For cases where any material may settle out of the spilled stream, it is necessary to include a sink term for that in the diffusion equation. Jobson and Sayre (44) and Sayre (9) describe inclusion of a sink term of the form

$$\text{sediment sink} = \frac{\partial}{\partial y}(V_s c) \tag{151}$$

in which V_s = mean fall velocity of a particle. This term assumes that settling of the solid particle removes that portion of material from the flow stream. However, as with sludge banks deposited on stream beds, they may either be reentrained or exert an influence from their new position.

In general, comprehensive kinds of sources and sinks are not included in the models allowing 2-D and 3-D diffusion. It will be necessary to define those forms proper to the materials of interest. In addition, realistic data must be available to describe the various reaction coefficients. Otherwise, the ability to better predict diffusion of material will be negated by poor treatment of the sources and sinks.

4. Initial Mixing - The only model mentioned where initial mixing is combined with diffusion is that by Caro-Cordero and Sayre (145), although a numerical model by Eheart (26) also attempts this. The ability to couple initial mixing in a convenient way with analytical diffusion solutions would be a big step. Even apparently non-jet behavior may have initial mixing as a feature. For example, Section I indicates that hydrazine is heavier than fresh water but lighter than sea water under most conditions. For discharges into freshwater, the tendency is for the material to plunge below the surface due to gravity. This density-induced velocity causes the discharge to first behave as a jet, with locally enhanced turbulent diffusion (often called entrainment) in the

early mixing. Eventually this density difference will be decreased through dilution with the ambient waters. About that point the plume will begin to be dominated by ambient turbulence and define a source location, size, and concentration for the diffusion solution. Any of the analytical solutions allowing a finite size source by spatial integration should be amenable to linkage needs to be accomplished and the combination put into a readily used form. Similar linkage could be provided in a numerical model such as that by Holly (115) by using a jet model to provide input into each of the stream tubes.

5. **General Review of Model Shortcomings** - The items mentioned as desirable are of course not all needed in every situation. However, a general model should have sufficient flexibility to be used in all possible cases. Of course, it might be necessary to prescribe more than one model for varying circumstances, but this is not the prefered arrangement.

Table 5 gives some pertinent information about several of the models reviewed so that a quick comparison can be made.

TABLE 5. A COMPARISON OF SOME AVAILABLE DIFFUSION MODELS

Model	Solution Technique	Dimension	u	h	B	Unsteady Source?	Finite Boundaries	Transverse Velocities Included?	Coefficients
Yeh-Tsai	Integral Transform	3-D	u(t): Eq. 5.4	Const.	Const.	Yes[a]	All	No	Questionable
Wang	Integral Transform	3-D	u(z,t)	∞	Const.	Yes[a]	Only B	No	Uncertain
Kuo	Integral Transform	3-D	Const.	Const.	Const.	Yes[a]	All	No	Inflated
Holley-Harleman	Images	1-D 2-D	u(t): Eq. 5.	Const.	Const.	Yes[a]	All	No	Std.
Prakash and Benedict	Images	3-D	Const.	Const.	Const.	Yes[a]	All	No[b]	Std.
Yotsukura - Cobb	Images	2-D	u(y)[d]	h(y)[d]	Const.[d]	No	All	Yes	Std.
Holly	Numerical	1-D	u(x,y)	h(x,y)	B(x)	Yes	All	Yes	Std.
Dailey - Harleman	Numerical	1-D	u(x,t)	h(x)	B(x)	Yes	All	No	Std.

Notes: a - By superposition and numerical integration; b - Can be included as constant v;
c - D_x approx. D_L; d - Can be made function of x also by segmenting into subreaches

It is apparent that the ability to formulate any time and space distribution exists using the super position principle, although a number of them have not been cast in those terms or would have to be programmed for that purpose. Some models include tidal advective velocities, but generally only allowing time variation. In the most elaborate of these, the Yeh-Tsai (135) model, there are questions concerning what coefficients are proper. In fact, this is one of the difficulties with several of the models even when the physical situation is well understood. The models by Holly (115) and Dailey and Harleman (78) are the ones most easily specified. The Yotsukura - Cobb (38) model has reasonable ability to predict coefficients, and this is increasing as more data is accumulated.

Initial mixing linkages may be feasible with any of these models, although the stream-tube models would be easiest, including Holly's. The image solutions would be next, with the integral transform solutions causing the most inconvenience. This all assumes that it might be necessary to apply the super position principle to a source of non-uniform concentration and hence cause bookkeeping problems in the computer programming. It could, however, be accomplished with any of the models.

Work will be needed to define and include proper source and sink terms. Boundaries are handled by all to varying degrees, with the most realistic being the stream tube models which incorporate arbitrary channel geometry, varying u, and bends.

It seems that there are a number of possible models, but no one model does it all. Some modifications or combinations will have to be made. In addition, a number of the new analytical solutions, such as Yeh and Tsai (135), which look so promising, need extensive theoretical investigation and sensitivity testing, as well as verification, to define constraints on their use and coefficient selection guidelines. Any model incorporating lateral and longitudinal

variations of velocity in rivers is preferred, because it reduces the number of items lumped into D_x, the single number most subject to error. In estuaries the lateral variation may not be so important due to the possibility that full transverse mixing may never occur, making D_x closer to Elder's $6hu_*$. In any event, further work is needed to define the best model and guidelines for its use.

SECTION VI
EXAMPLES OF MODEL BEHAVIOR AND CHARACTERISTICS

OBJECTIVE

The ability to see numerical examples is frequently helpful in understanding the impact of certain assumptions, parameters, or model elements. For this reason, a number of simple examples have been generated on the computer for illustration purposes only. They are not intended to represent a completely arbitary situation, but rather one example. In addition, they are not intended to represent any form of sensitivity analysis. Such analysis will have to be an integral part of testing, verifying, and documenting any model or models finally selected.

In reading this section, one should note that often very similar effects can be given by different physical features of the system. Therefore, any attempt to use a model to evaluate, e.g., a decay coefficient, would be subject to error due to any error existing in other parameters.

Unless specific mention is made otherwise, the results shown in this section were all generated by use of the image solutions given by Prakash (109), as modified by Benedict (110). This model was selected due to the relative ease of programming as compared to, say, the Yeh-Tsai (135) model, which would have required a programming effort beyond the scope of the current work. In most cases, values taken from the paper by Prakash (109) for use in some of his numerical examples are used here. They are for a reasonably large river and indicate a reasonably high level of lateral diffusion. These values are listed here, and when different values are used, they will be noted at the point of discussion.

TABLE 6. COMMON PARAMETER VALUES FOR EXAMPLE

Parameter	Value
B = stream width	2100 feet
h = stream depth	19.5 feet
u = stream velocity	2.71 feet/seconds
Q_o = release rate of fluid containing tracer	3598 gallons per minute
C_o = concentration of tracer fluid in Q_o	1500 parts per million
D_y = transverse diffusion coefficient	8.2 ft^2/sec
D_z = vertical diffusion coefficient	0.082 ft^2/sec
D_x = longitudinal coefficient	varies

A few thoughts concerning the coefficients are in order. If one assumes that $u/u_* \simeq 0.1$ [(see Equation (33)] then α [(from Equation (32)] is about 1.6 for D_y and 0.016 for D_z. The former is the range of values reported in reaches with bends, while the latter value is lower than the generally accepted 0.067 [(Equation (35)]. In a design situation, 0.067 is recommended unless buoyancy forces are expected to lower D_z. Here, Prakash's value is used to facilitate comparison with some of his examples. For reference, Elder's value of $6hu_*$ for D_x due solely to vertical variation of longitudinal velocity would range from about 15-35 ft^2/sec over expected possible ranges of u/u_*.

EFFECT OF BOUNDARIES

Boundaries are relatively easy to understand in their influence. When they begin to play a role, they increase the concentration above that which would exist at the same point with no boundary. This is true physically because of the shortage of dilution water. Mathematically, one can look at the method of images formulation and visualize material being reflected back into the finite flow space. To illustrate this effect, Equation (124) was used to generate the results shown in Figure 14 for a continuous plane source of width 150 feet and depth 3 feet. This could perhaps occur due to a pipeline rupture, a gash in the side of a barge, or other causes. In Figure 14, results are shown at the bank (y=0) at the water surface (z=0). In one case, the river width, B, is 500 feet and in the other it is 2100 feet. Notice that the influence of the

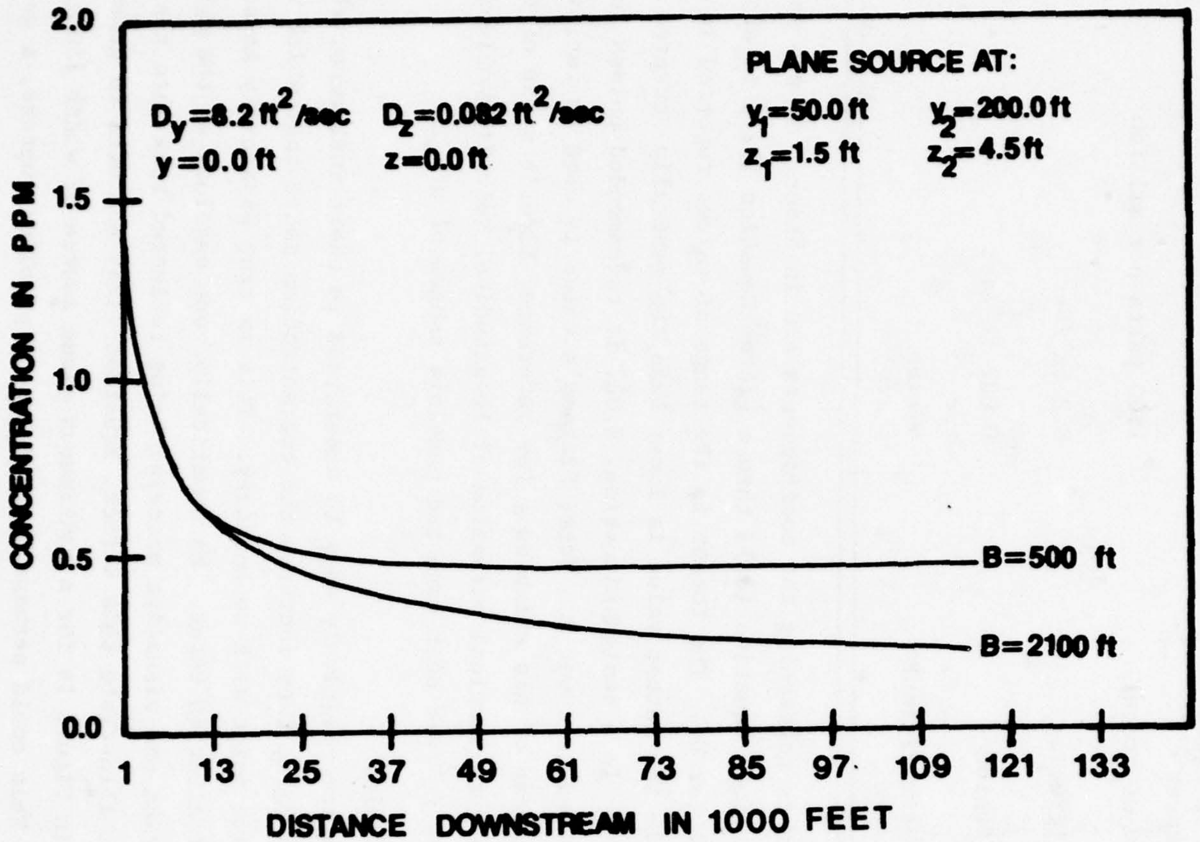

Figure 14. Effect of Stream Width on Mixing

boundary is not even felt for about the first 13,000 feet. Note that results have been extended downstream about 25 miles, although this length often would require segmenting the river.

EFFECT OF DECAY COEFFICIENTS

The effect of a single first-order reaction of the form $-\lambda t$ has been included in a number of the equations and usually appears as a multiplier of the form $\exp(-\lambda t)$ for instantaneous releases or $\exp(-\lambda x/u)$ for continuous releases. The term x/u gives some measure of the time of travel from the release point to the point of interest. This means essentially that the $\lambda = o$ concentration at any point downstream is merely multiplied by the proper term. Figure 15 shows the same example of a plane source shown in Figure 14 for three different λ values, 0, 0.1, and 1.0 day $^{-1}$. These are of the order of typical decay coefficients often assigned for BOD, for example. Note, however, the key fact that here, where 3-D mixing is going on, the primary mode of reducing concentration is through the dilution due to diffusion mixing, not the decay of BOD. In a 1-D continuous discharge case, where longitudinal dispersion is often insignificant, then the decay would be the only mechanism, as illustrated in Equation (92). It is again interesting to note that errors in describing the advective or diffusive terms could easily mask the differences in λ shown. Again, in other cases where the role of the reaction term is greater, this might not be the case. Also, notice some similarities between Figures 14 and 15. The effect of widening the receiving body and removing some boundary influence can have an effect comparable to increasing λ. For this reason, λ should always be evaluated based on laboratory chemical or biological analysis, rather than by fitting to diffusion solutions.

INFLUENCE OF LONGITUDINAL DISPERSION

Considerable discussion has been given to the longitudinal coefficient,

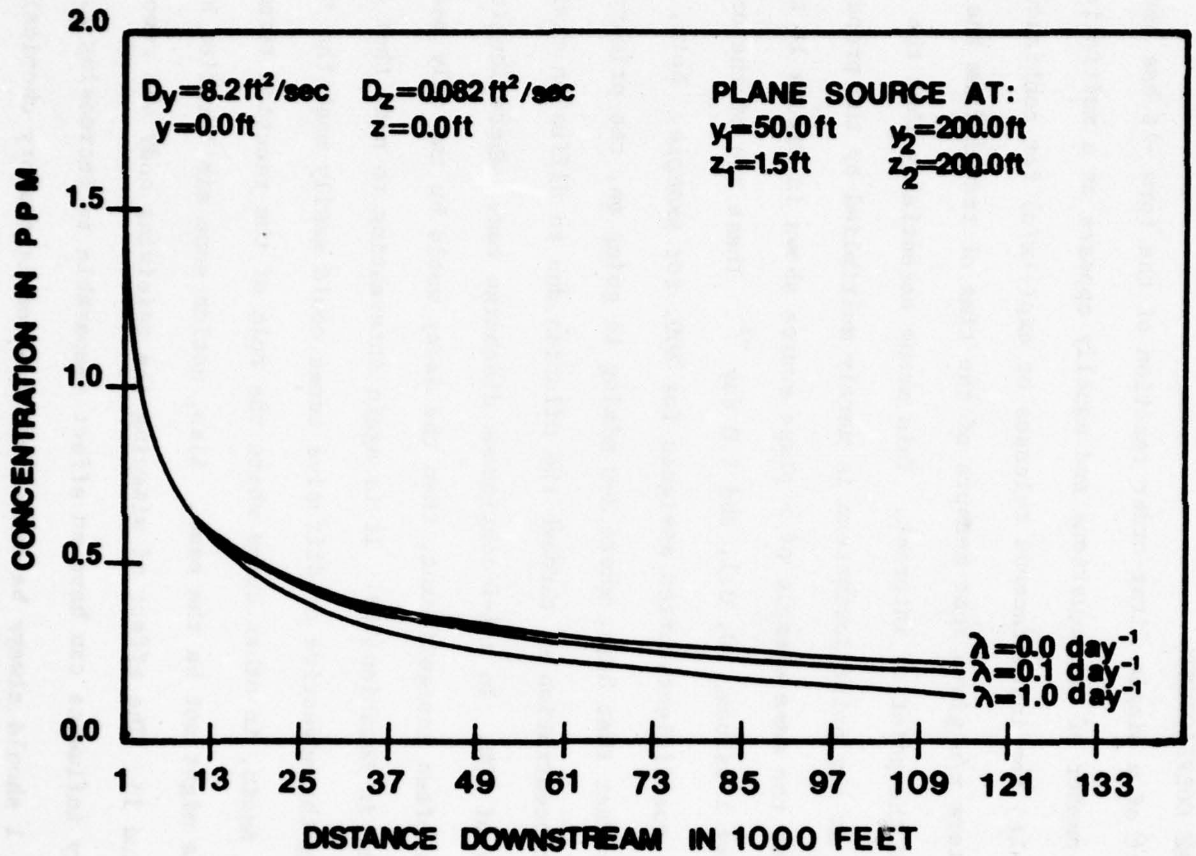

Figure 15. Influence of Decay Coefficient

D_L or D_x, and what it includes in different models. It has been indicated that in continuous discharge situations, the D_x contribution can be neglected except very near the source. An example of a criterion for near is given in Equation (89). However, few spill problems will become continuous, and therefore proper selection of D_x becomes important. A simple example using the same plane source as in Figure 14 and 15 shows some interesting features.

Three separate D_x values were selected, ranging from 2500 ft^2/sec to 10,000 ft^2/sec. Notice that this implies that D_x/hu_* ranges from about 600 to 2400. Figure 16 shows the effect at a single location (x,y,z) and (1000, 120, 0 feet) for a discharge continuing for 90 minutes, or 5400 seconds. Notice that the concentration builds up with time and has approached very close to a steady state condition for all three cases. This is not surprising when one realizes that the mean travel time (x/u) to this point is 1000/2.71 = 369 seconds and 5400 seconds is about 15 times this long. If the discharge continued a bit longer, all three would reach a plateau of constant concentration. The final values would be different for all three cases. If the discharge were halted prior to 5400 seconds, then the curves in Figure 16 would reach a peak lower than the steady-state plateau and then fall off.

Note that the concentrations decrease as D_x increases. This is because a higher value of D_x implies that material is being spread out longitudinally at a higher rate due to velocity variations within the section. One can view each instantaneous slug of material as being spread out while it is being advected. For a higher D_x, more of the material has passed the point x=1000 feet by the time other slugs are felt there. Recall Equation (89) for the distance to the point where D_x can be neglected for a continuous vertical line source. Use of this as an approximation, it can be seen that minimum distances for neglect of D_x would be range from 1845 feet to 7380 feet. Therefore, x=1000 feet

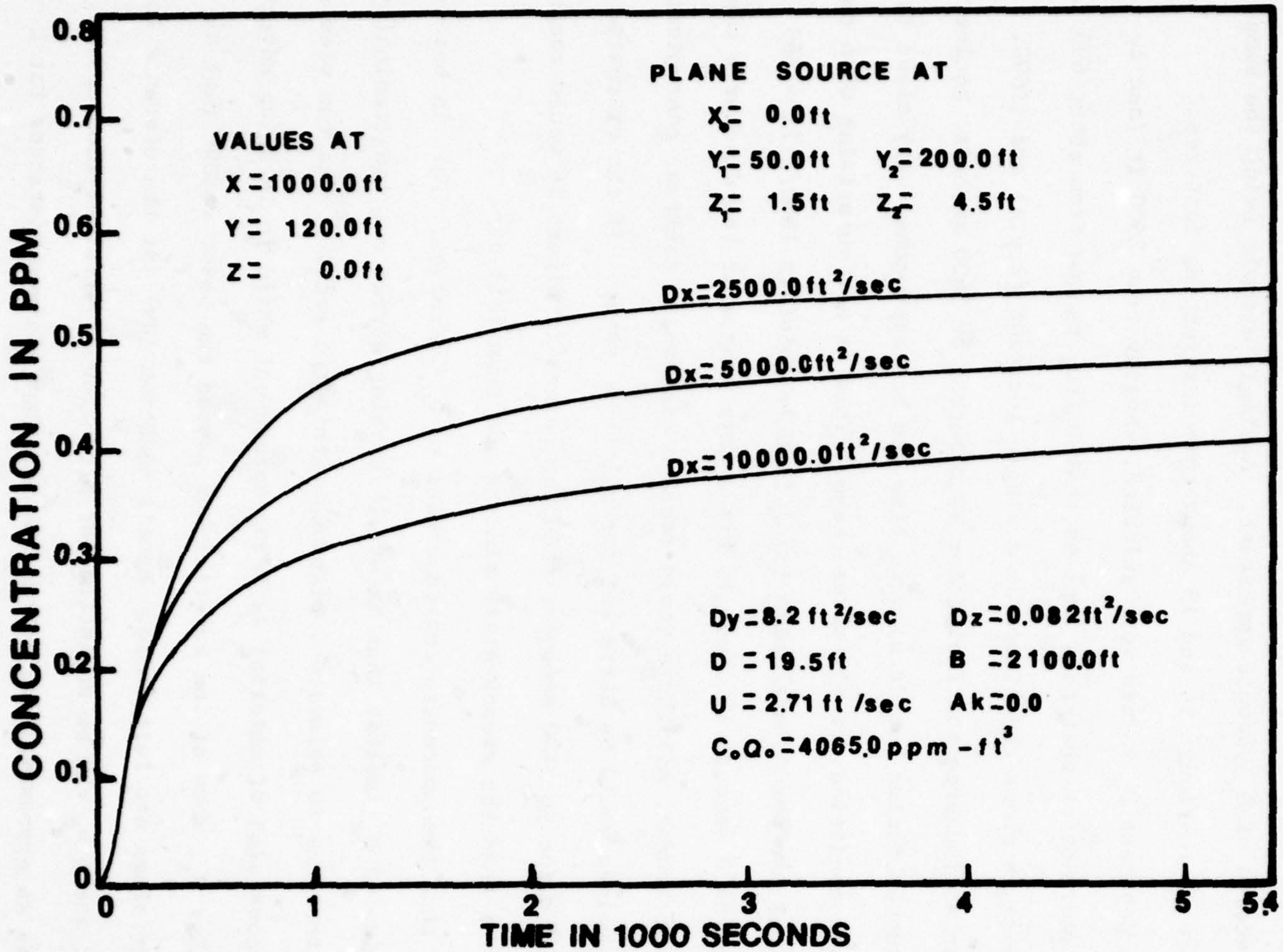

Figure 16. Temporal Variation of Effect of Longitudinal Dispersion

is much less than these, especially for the higher D_x values. It can be seen that even if the discharge were continuous, neglect of D_x would not be proper if it were believed to be in the indicated range. Much further downstream, differences would become negligible.

Figure 17 gives another view of the same solution, looking at the concentrations downstream at a given instant of time, specifically at the instant when the discharge is discontinued. The mean distance traveled by the first slug (t=o) would be 5400 (2.71) = 14,630 feet. Shortly past this point, the curve for 2500 ft^2/sec begins to fall of more rapidly and ultimately the curves cross. This is because any material existing past 14,630 feet had to reach there by dispersion, not advection. The larger D_x value spreads the material out more, hence leading to the cross-over.

These examples help illustrate the importance of D_x. Even if the discharge is deemed continuous, some minimum distance is required before D_x can be neglected. If a critical point of potential damage is within that distance, then neglect of longitudinal mixing could be significant.

SKEWED VELOCITY FIELD BEHAVIOR

Related to longitudinal dispersion is the shearing action due to a skewed or non-uniform velocity field. The vertical line source Equation (118) was used to compare with Monin and Yaglom's (105) model, as shown in Equation (148). A simple instantaneous release was modeled for a line source over the fluid depth, and two separate reviews were made.

1. c vs t for (x,y,z) = (1000 feet, 0,0)
2. c vs y for x = 1000 feet, z = 0, t = 360 seconds

It is assumed that 1800 gallons of liquid is spilled, and the material of interest is contained within this liquid at a concentration of 1500 ppm. One case was chosen with a uniform velocity field, u = 2.71 feet/second everywhere; the second was selected with Γ_y = 0.004 feet/second /foot. The coefficients are

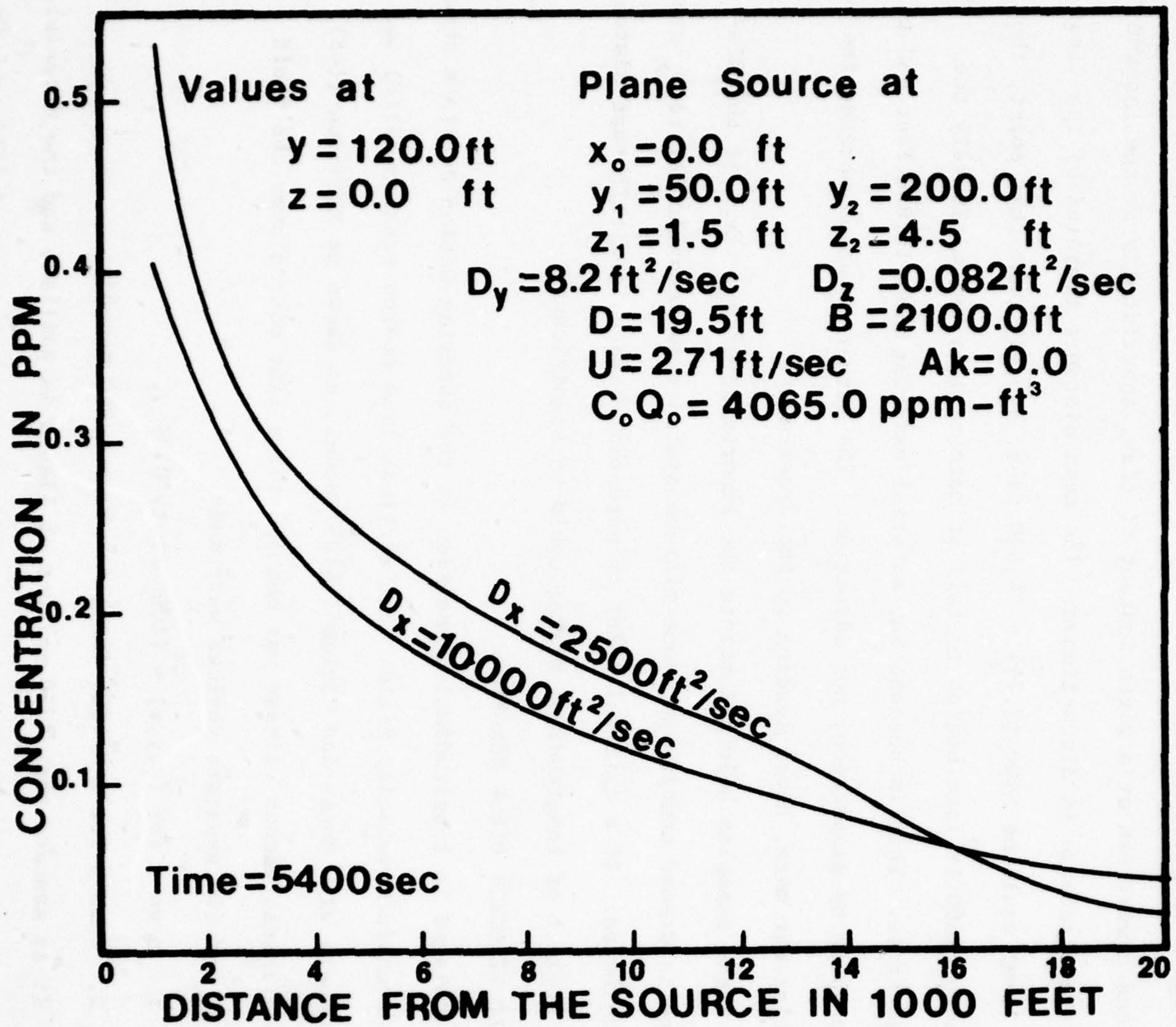

Figure 17. Spatial Variation of Effect of Longitudinal Dispersion

selected as $D_x = 25\ ft^2/sec$ and $D_y = 10\ ft^2/sec$.

The c versus t curve for the skewed and uniform distribution varied as expected, but differences were too small to detect on a graph. In general the c versus t curve for the skewed field rose slightly more rapidly, had a slightly lower peak, and tailed off more slowly. Notice that this is exactly what would be expected if a higher D_x had been used. This is expected, for the skewed velocity field imposes dispersion on the spreading incorporated in the single, constant D_x.

Figure 18 shows the second item, lateral distribution of c at x=1000 feet, t=360 seconds. The skewed distribution is only slightly lower at the channel center, where U_o=u=2.71 feet/seconds, but the concentration falls off much more rapidly than for the uniform distribution. Recall that this was a single slug instantaneous release. In the region where $u>U_o$, the cloud is moving faster than the corresponding cloud in the uniform field; therefore, concentrations are less with the skewed distribution because a larger portion of the cloud has already passed that point at t=360 seconds. On the opposite side, the reverse is true. The concentration there is lower because the material is moving more slowly and not as large a portion has yet arrived. Notice,however, that the two sides of the skewed distribution are not symmetrical, as Okubo and Karweit (151) discuss. Concentrations are higher in the region of higher velocity. In fact, Okubo and Karweit (151) show the results of a continuous discharge in the same form as Figure 18. The continuous discharge represents superposition of an infinite number of instantaneous release. The elements seen in Figure 18 would be accented, with the skew becoming more pronounced, and, if Γ is large enough, the peak will be located reasonably far into the higher velocity region.

This subsection has merely tried to point out the importance of the velocity field in making diffusion predictions. The skewing of the distribution

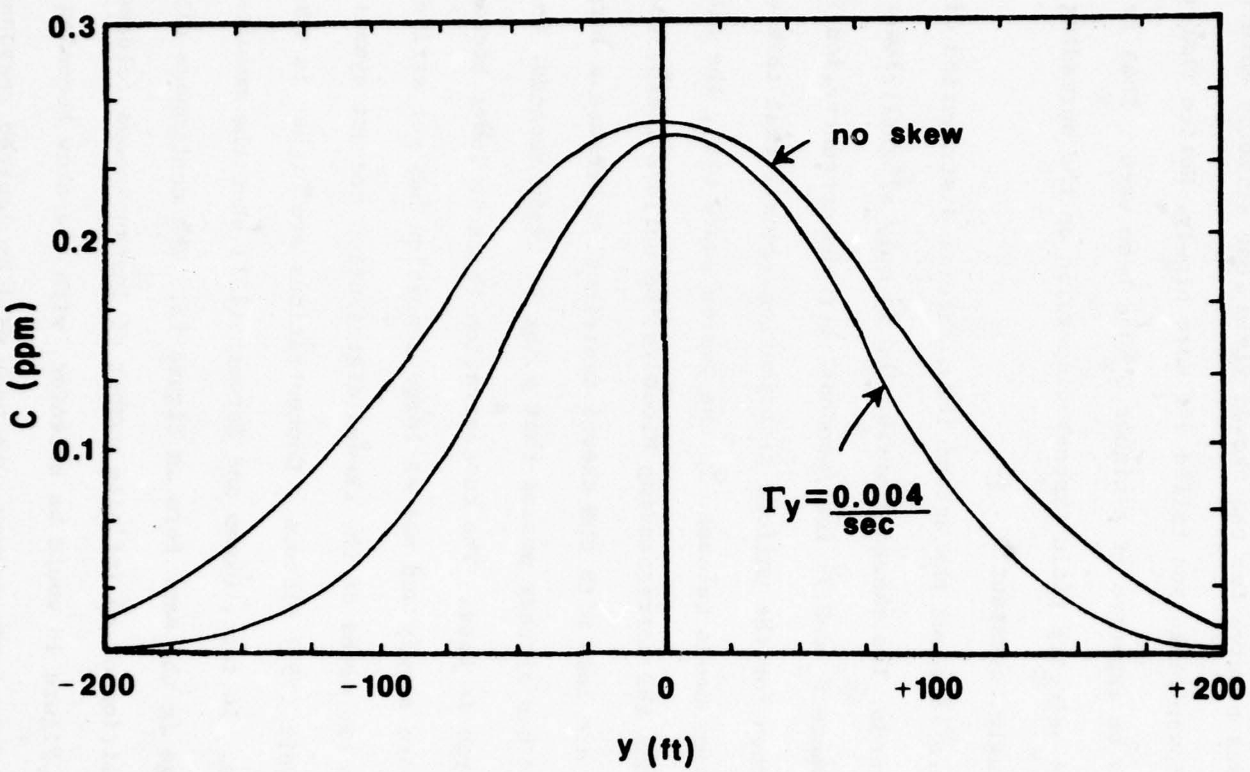

Figure 18. Effect of Velocity Shear

to the higher velocity regions helps in understanding plume behavior around bends and in non-uniform geometry. It further underscores the need for inclusion of as much advective information as reasonably possible in a model.

INFLUENCE OF SOURCE CONFIGURATION

Section IV discussed the variety of spatial conditions which may be used to describe a source. An immediate question concerns the accuracy needed in source specification. Does use of a point source approximation rather than a volume source cause problems, for example, and if so, when and how much? Answers to these questions deserve definitive answers. A couple of numerical examples are presented here to illustrate the types of things to review.

A comparison of Equations (82) and (125) shows that as the size of a volume source is assumed larger, the initial concentration in the water becomes smaller. This will lead to lower predicted concentrations near the discharge point. For example, consider a spill assumed to initially occupy a volume of a one foot cube. If the same material were instead assumed to be spread, initial concentration of the latter case is only one percent of that in the former. Review and testing of Equations (82) and (125) indicates that no matter what the discrepancies initially, at sufficient distance downstream the effects of initial source size are masked out by the mixing processes and results are indistinguishable. The unanswered question is what is a sufficient distance.

As an example, consider a spill released instantaneously at time zero. For one spill rate, stream velocity, depth, etc., three different source conditions were assumed and compared using Equations (82) and (125) and the corresponding equation for a plane source Equation (122). The table shows peak concentrations obtained at x = 1000 feet downstream. Values were as shown in Table 7 , with D_x = 234 square feet per second.

TABLE 7. EXAMPLE OF SOURCE EFFECT
FADING WITH DISTANCE AT X = 1000 FEET DOWNSTREAM

Source	Peak Concentration,ppm
Point at channel center	0.874
Plane: 3 ft x 150 ft from y = 0 to y = 150 from z = 8.25 to z = 11.25	0.843
Volume (1.6 ft x 50 ft x 3 ft) x = 0 to x = 1.6 y = 50 to y = 100 z = 8.25 to z = 11.25	0.874

For practical purposes, no real differences exist at this point. At shorter distances, nearer the source, discrepancies can become significant. For other sets of parameters, concentrations might not approach so closely for a much longer distance.

Figure 19 shows a further example, this time for a continuous discharge. A point source and two separate plane sources are selected through which to assume the same material flow rate occurs. In the first few thousand feet, some values differ substantially. However, by 2 to 3 miles downstream, differences are small when compared with other possible errors. Notice once again the similarity between the curves in Figure 19 and those in Figures 14 and 15. The differences due to assuming different source conditions are similar to those due to boundary constraints and decay, at least in appearance in the predictions.

It is obvious that in many instances the exact spatial source characteristics may not be too critical. However, if potential trouble areas (such as water intakes, recreation areas, fish breeding grounds, etc.) are very close

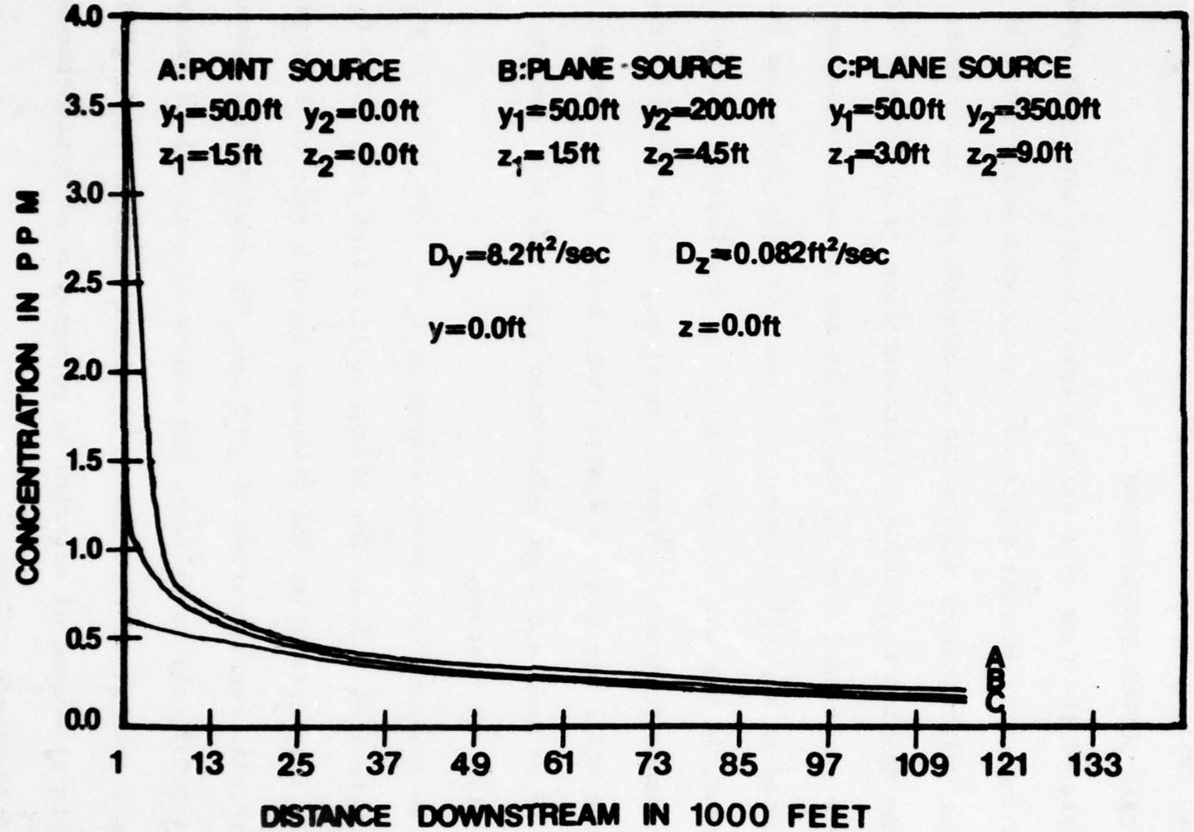

Figure 19. Comparison of Three Sources

to the spill, proper selection of source conditions becomes very important. Even the use of a point source may not assure a conservative, over estimated concentration. Assumption of a point source when a finite size source actually exists will cause prodiction of too small a plume in the region near the source, possibly failing to show plume interaction with some critical area.

EFFECT OF TEMPORAL SOURCE DISTRIBUTION

The estimate of the time over which a spill occurs can be important in predicting its impact or in attempting to compare with known data. An estimate of the time over which leakage occurs can be coupled with an estimate of the total volume spilled to provide a representative value for the discharge rate. If only a worst case view is sought, it may be well to assume all the material is dumped at a single instant of time. If this indicates acceptable levels downstream, it may not be necessary to go any further. However, if this simple estimate indicates potential problems, and if there is reason to believe that the spill may cover a finite time, then a better estimate of that time should be made and a new assessment made. In the same way, refinement of the source size can proceed.

Consider an example for a plane source at x_o=0, from y_1=50 to y_2=200 feet, and from z_1=1.5 to z_2=4.5 feet. The stream is 19.5 feet deep, 2100 feet wide, and flows at 2.71 feet/seconds. The discharge is at a rate of 3598 gallons/minute, with an initial concentration of 1500 ppm. The coefficient values are D_x=234, D_y=8.2, and D_z=0.082, all in ft^2/sec. The amount of material is assumed equal to that discharge at the given rate over a 30-minute period. It is then assumed that the same total volume of material is released as an instantaneous release and as a 10-minute release.

Results are shown in Figure 20. Here, the peak assuming an instantaneous release is obviously worse than the other two cases. It is conceivable there might be times, however, when exposure time is a factor in assessment and a

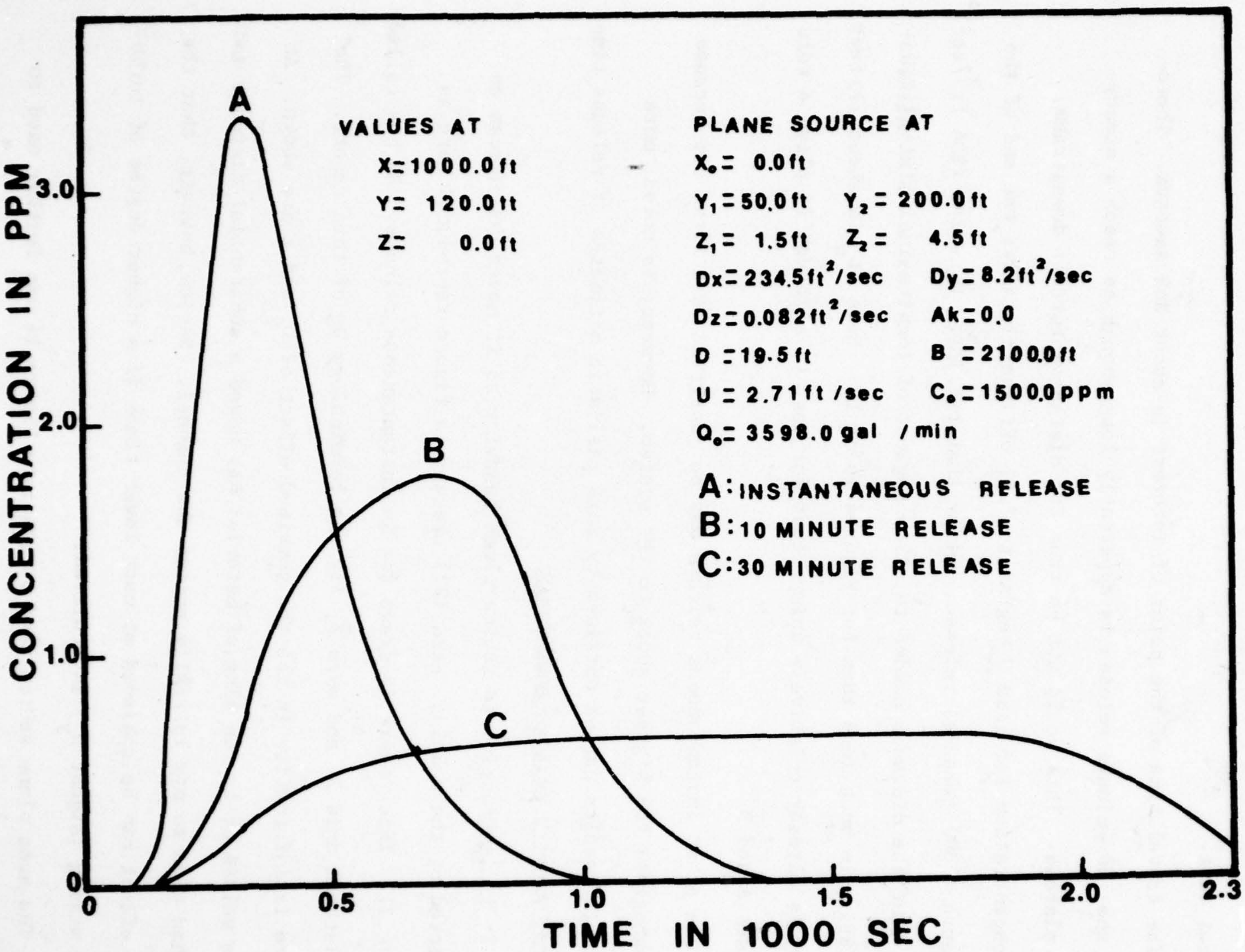

Figure 20. Comparison of Three Release Intervals

lower concentration which is maintained for a long time might be the most cr critical case.

The travel time of the point of interest is about 369 seconds. Therefore, the 30 -minute release is apparently long enough to reach a steady-state plateau. This would not be true for distances further downstream. The concentration for case C begins to fall off shortly after the end of the 30 minute (1800 seconds) release. Notice that the lower D_x value (234 ft^2/sec) means that the distance needed to allow neglect of longitudinal mixing [(Equation (89)] is much less than for Figures 16 or 17. Here L_n is about 175 feet, and D_x is already relatively unimportant for case C, although it plays a role in cases A and B.

Use of an instantaneous release may be justified as a first cut because it represents the biggest shock to the system. However, as noted, more realistic results can be obtained by more realistic estimates of release time.

TYPICAL PROFILE CHANGES DOWNSTREAM

It is instructive to review plume behavior as it moves downstream as predicted by the models. Ward (97) presents a figure reproduced here as Figure 21. This figure is drawn for an instantaneous release. He has called the lateral axis Z and uses $\bar{E}_z$ for the terminology D_y of this report. The figure is informative in the the combined effect of D_y and t are shown. At large values of t, the slug of material has moved a substantial distance and has had time to mix laterally across the channel. Notice, however, that the same effect can be achieved at much lower times if a higher degree of turbulent mixing (higher D_y) is achieved.

The same plane source used to generate Figure 14 was further used to review vertical and transverse spreading of the resulting plume. Figure 22 shows lateral profiles of concentration at three downstream locations, while Figure 23 shows the vertical proviles at other locations. Note the strong

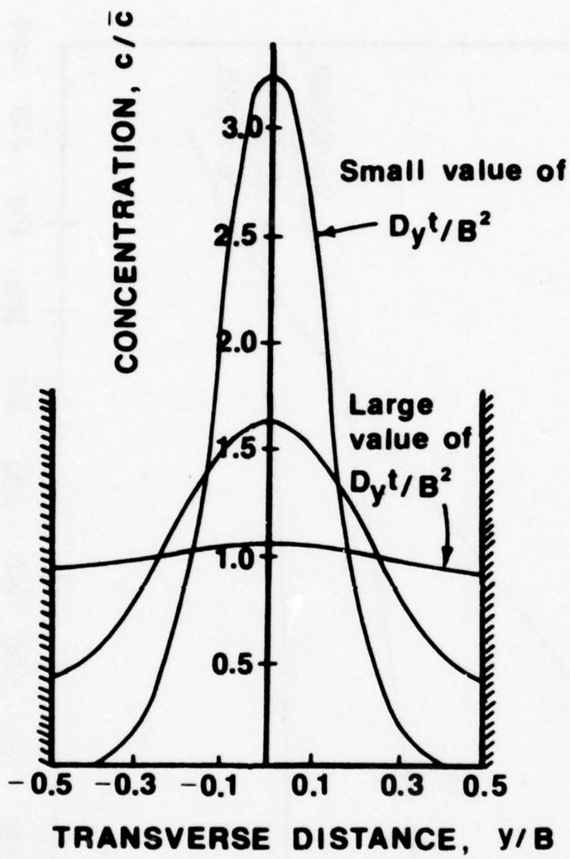

Figure 21. Profile Variation Downstream [After Ward (86)]

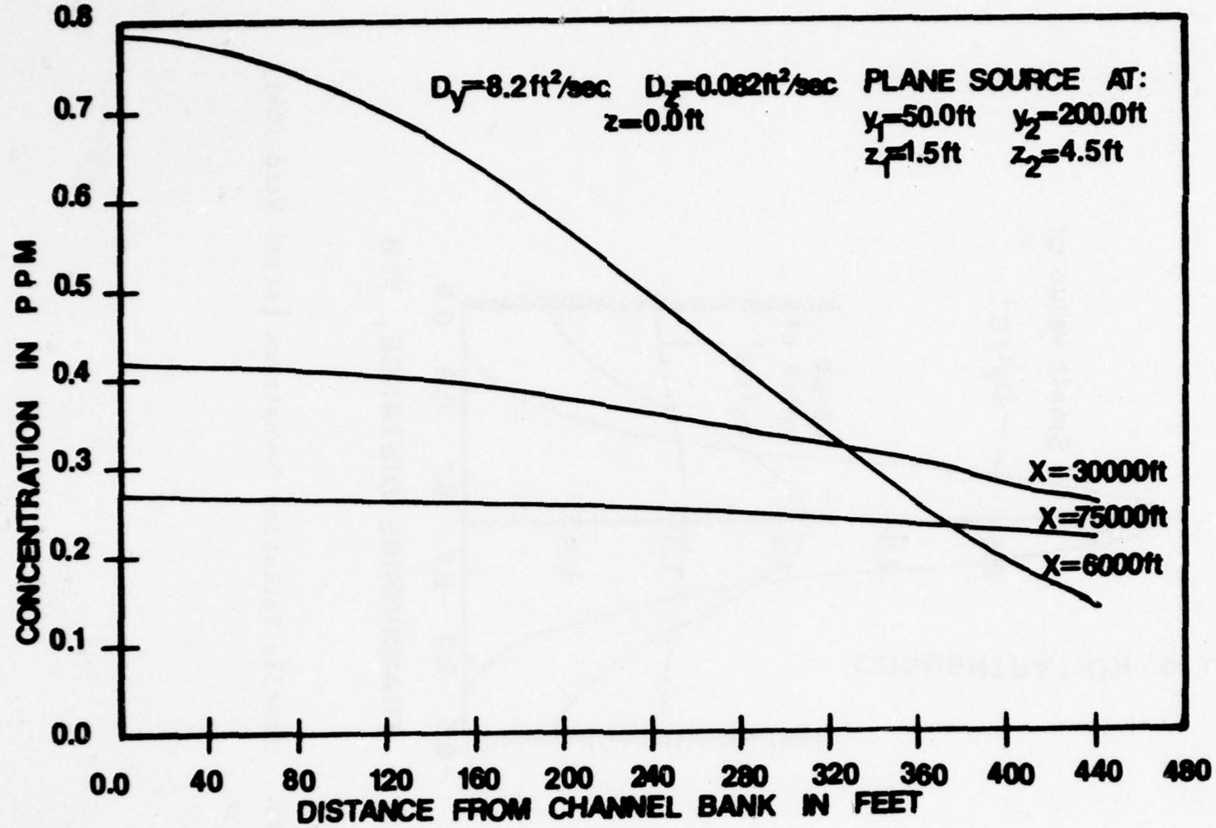

Figure 22. Changes in Transverse Concentration Profiles with Distance

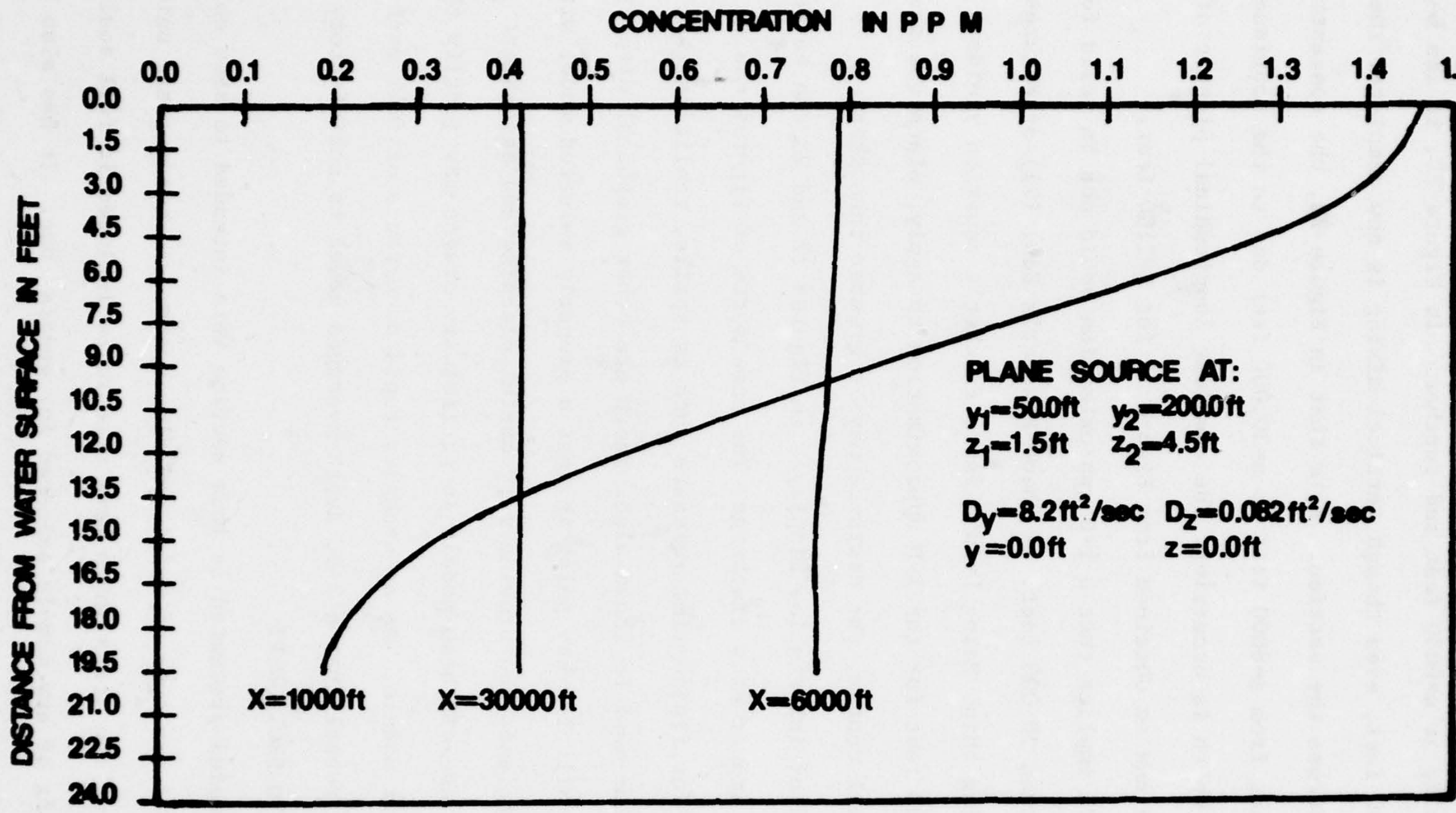

Figure 23. Changes in Vertical Concentration Profiles with Distance

vertical gradient at x=1000 feet in Figure 23, while the tracer is completely mixed vertically at x=6000 feet and further. In Figure 22, it can be seen that at x=6000 feet, even though vertical mixing is now complete, there is still some change across the section. Note that in Figure 23, the concentration drops in moving from x=6000 feet to x=30,000 feet due to the continued transverse mixing which is occurring. The complete longitudinal picture of behavior of this plume can be obtained from Figure 14 for B=2100 feet.

Figure 22 implies that a 1-D approximation would not be valid for distances less than 30,000 feet, if then. Fischer's Eqn. (71) or Figures 7 and 8 enable checking this. Using L=1050 feet, Fischer's equation yields a length, x_I, of 145,000 feet for the 1-D approximation to apply. Since the source is off the channel center, the distance may be greater than this.

The kind of information displayed in Figures 22 and 23 can be very useful in assessing impact of a discharge. The same sorts of figures can of course be generated for finite time releases such as spills, realizing that the variation with time must be shown also. There are other graphical display possibilities as well. The key point is that a properly selected model with carefully chosen coefficients can provide very useful planning and assessment information. In addition, use of these models in preliminary stages may justify the possible use of simpler models. As an example, rapid occurrence of full vertical mixing might reveal that a 2-D, depth-averaged model is satisfactory.

CONCLUSIONS TO SECTION VI

The examples presented in this section were intended to show only characteristics of one type of model and flow system, a steady-state unidirectional flow. Some of the items shown here need to be included in full scale sensitivity testing of any models selected for general use. It has also been seen

that occassionally more than one physical change might induce the same type of observed change in mixing behavior. All of this points toward using a model which eases problems with specification of input parameters.

SECTION VII

RECOMMENDATIONS FOR FUTURE WORK

This report has attempted to summarize the status of models which might be applicable to Air Force assessment of possible impact due to toxic spills. Problems with models were reviewed, with special emphasis being given to those which were likely to cause problems in model application. An example is the tendency to lump much advective behavior into the diffusion and dispersion coefficients. All of this discussion leads to the conclusions in Section V, specifically that no one available model can currently be considered generally applicable to spills of toxic materials. The following suggestions are offered to guide work in development of a final model package.

CRITERIA TO BE ESTABLISHED

It is clear from the earlier sections that there are frequent questions as to the applicability of certain models or features. Some criteria have been offered for certain of these, but they must be refined to assure effective decision making when Air Force personnel employ the model or models. A few are discussed here.

1. Longitudinal Dispersion - The criteria offered by Sayre and Chang (10) in Equation (89) is valid for a line source and gives an estimate of the distance one must go downstream before longitudinal dispersion can be neglected for a continuous discharge. Thomann (39) has offered objective criteria for neglect of D_L, but only in the 1-D equation. A general criterion needs to be established to insure that, at the least, the proper level of effort goes into defining D_x (D_L). This criteria should fit all sources.

An additional element for consideration is the definition of D_x itself in the cases where transverse averaging of the longitudinal velocity has occured. In the case where the plume does cover the entire stream width,

the plume is exposed to the entire lateral spectrum of longitudinal velocities. If this happens, then D_x is probably close to D_L in value. However, in the event that a plume covers only a portion of the stream width, only that portion of the stream in which the plume exists should be included in the velocity field averaging process. This may lead to greater or lesser D_x values depending on the gradients within the plume.

2. Selection of Source Conditions - It it is possible to better define criteria for selection of the spatial and time distribution of the source, this should be done. This can partially be accomplished by objective criteria indicating times and/or distances after which certain source characteristics become unimportant. Guidance to selection of a source size can be more effectively presented by a review of possible initial mixing, which should appear in the final model.

3. Better Coefficient Guidelines - This report has attempted to summarize coefficient knowledge as it exists today. Once a final model or models are developed, it can be determined exactly what advective behavior is included in the coefficients. This can be done by comparing the equations term by term and carrying out necessary integrations. Once the coefficient characteristics are known, selection guidelines should be established as precisely as possible. It is understood that a knowledge of the physical site is essential to the best judgement, but it will frequently be possible to use only easily obtained data on size, flows, etc. The guidelines should be established so as to recommend values (or procedures to obtain them) for every case of model application, with warnings for special cases and suggestions to obtain conservative results where real uncertainty exists. Sensitivity testing (mentioned later) of the model will be essential to provide guidance on the accuracy required of the coefficients in typical applications.

MODEL MODIFICATIONS AND ADDITIONS

There are some elements which should be included in any model unless further study reveals that it is too complex in certain situations. A few are presented here, and sources and sinks are discussed in a later section.

1. Initial Mixing - In some instances, it will be clear that some initial mixing occurs, where momentum effects of the discharge create locally enhanced turbulent diffusion, often called entrainment when jet mixing theory is applied. Proper selection of source configuration should include this mixing. Sayre and Caro - Cordero (22) have done so by using previously published empirical formulas to estimate dilution prior to the diffusion region beginning. This may be a reasonable beginning point, although little work has been done on initial mixing for instantaneous or other non-continuous releases. This could also possibly be handled by segmenting the model to allow for varying coefficient values in the initial mixing region. A proper means for simple, effective inclusion must be sought. In addition, momentum effects due to buoyancy (hydrazine, e. g., is usually heavier than fresh water, lighter than salt water) must be included.

2. Inclusion of Channel Bends - The influence of channel bends and their resulting transverse currents and wake regions present a significant problem. Two elements to the problem include (1) enhancement of mixing over longer reaches and (2) extreme variations in mixing behavior according to position in the bend, both longitudinally and laterally. A way to include these features in a model must be developed, either by use of the model in connected subreaches of the river or by inclusion through some stream tube model.

3. Spatial and Temporal Variation of Coefficients - Most of the models discussed herein have utilized constant values for the coefficients. However, these values may vary both spatially, and, when receiving water flows are

unsteady, temporally. At this time, it is difficult to define what form these variations will take. However, the most useful model would be one allowing for rather general functions describing these variations. It may turn out that mathematical convenience will be worth more than this generality, but it should be investigated. Some means of handling the problem of local variations in bends should be investigated.

ARBITRARY VELOCITY AND GEOMETRY VARIATION INCLUSION

Discussions of the "natural" coordinate system, cumulative discharge, and stream tube models in Sections II and V have shown that some simple uniform, steady flow cases can be solved with the velocity input as a function of transverse location. Holly (115) prepared a numerical model for steady flows including channel non-uniformity proceeding downstream. Yotsukura and Sayre (38) note the use of segmenting the river to allow for non-uniformities. Some means of correctly including as much of this information in the final model should be found.

INCLUSION OF OTHER SINK AND SOURCE TERMS

The only sink shown in this report is one for a first-order reaction. Many models include this because it is easy to obtain mathematically. However, some others may be pertinent, and any future work must be required to coordinate with Air Force personnel on their best knowledge of hydrazine (or any other material of interest) behavior.

1. Sedimentation - If any of the materials of interest may contain solid particles in suspended form, or may adsorb on suspended sediment in the receiving stream, then a term should be included in the model to account for settling out of material. If the material may continue to exert an influence from the streambed, this should also be included.

2. Dissolved Oxygen Effect - Any toxic material is likely to exert a demand on oxygen resources in the stream. If this is expected, then the coupled

equation for oxygen, with its other sources and sinks as well, must be included. Proper input of reaction rates will have to come from laboratory work.

3. Other Secondary Factors - In addition to dissolved oxygen, hydrazine or any other material may have an effect on other constitutents in the stream. The term secondary is used to apply to any constitutent other than the spilled material itself. Changes in other constituents in the receiving water can be harmful. Such constitutents should be identified by consulation with Air Force personnel and built into properly coupled equations in the model.

4. Staged Reaction Rates - It may be that the material exerts a sudden, immediate demand on some material such as oxygen and then uses it at some slower rate as the plume proceeds downstream. It may also be that the reaction coefficient is concentration dependent. In these cases, it will be necessary to investigate ways to allow for various stages of the reaction rates in the model.

VERIFICATION OF MODEL

The word verification is perhaps misleading. It is unlikely that sufficient data will exist to adequately verify the model for all conditions. However, numerous field investigations have been conducted, as well as laboratory studies. The model should be shown to reasonably match data for a number of cases typical of spill situations using the coefficient selection guidelines given in the final study. This process will likely require careful review of the actual testing procedure in order to specify proper source conditions. In addition, it may mean using a model with 3-D diffusion for analysis of data other have treated as 1-D.

SENSITIVITY ANALYSES

A thorough sensitivity analysis of the model should be made. It will be necessary to accomplish some of the other suggestions, including setting

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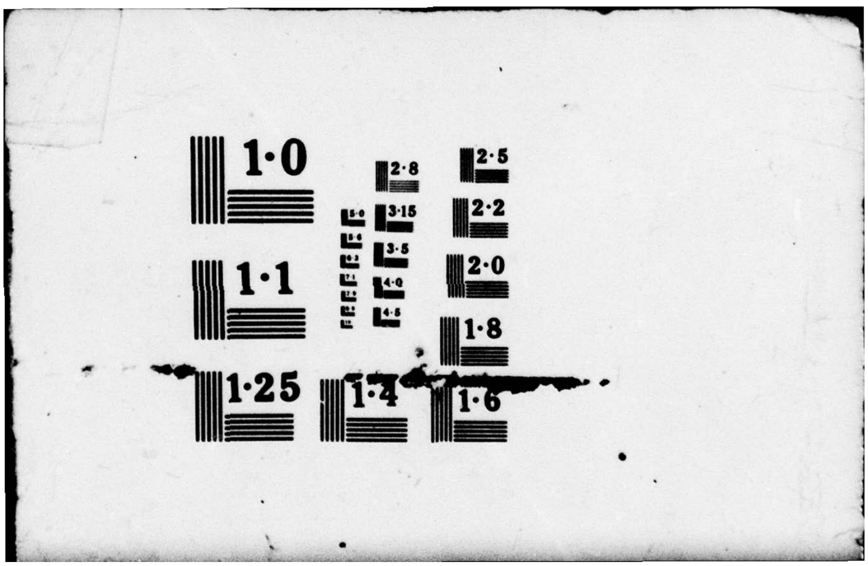
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coefficient selection guidelines. However, it will also be necessary to properly understand model behavior and suggest errors in concentration predictions which might be associated with given input errors and help establish some confidence bands in certain cases. The results of the sensitivity testing should be used to describe those situations where dangers may occur and, on the other hand, those cases where less care is needed in defining certain inputs.

MODEL DOCUMENTATION AND USE

It is suggested that the model or models finally selected be documented fully to enable use by others conveniently and securely. It is suggested that improved output formats be considered, including possible attempts to generate plots of isoconcentration lines in the plume as the spilled material moves downstream. Finally, specific examples (with hydrazine for example) should be presented in a variety of cases to assure that the general user can utilize the package.

GENERAL COMMENTS

The modeling of diffusion and dispersion processes is not a static field. New information is always being developed. It is expected that the final model developed should be capable of incorporating new material as it seems valuable. The major goal should be to provide a tool which can be applied inexpensively and conveniently to any circumstance without having to have a diffusion and dispersion expert watching every step. It is believed that this can be achieved if the warnings contained in this report are heeded and if care is given to define model use and limitations.

SECTION VIII

CONCLUSIONS

SCOPE

The work presented in this report is intended to review techniques for modeling possible spills of toxic materials. Basic methodologies and available models were reviewed with the goal of assessing their usefulness and shortcomings for Air Force use. The ability to select coefficients for use in the various models was also reviewed, due to their significance in the prediction of spill behavior. Examples of model output were presented to illustrate typical behavior and model performance. The review enabled recommendations for future model development to provide a useful planning and assessment tool for the Air Force.

BASIC EQUATION DEVELOPMENT

The basic convective-diffusion equation includes all advective terms. However, averaging the entire equation or one or more terms over the width of the water body, the depth of the water body, or over some time frame removes some of the advective behavior from the equation. Essentially, anything other than some mean behavior is neglected. This neglected behavior reflects itself in changed values for the diffusion coefficients. Thus it is important to know the characteristics of the equation to properly select coefficients.

It is observed that some of the neglected behavior around bends, as well as lateral averaging of the equation, can be overcome by use of a natural coordinate system, as outlined by Yotsukura (32), and replacement of the lateral dimension, y, by the cumulative discharge, q, as the independent

variable in the diffusion equation. Yotsukura and Cobb(36) proposed this change, which implicitly incorporates transverse velocities into the equation.

COEFFICIENT VALUES

Having established the effect of equation development on coefficient values, it was deemed necessary to review the physical features influencing those coefficients. The basic formulae for coefficients are defined, specifically the shear velocity representation in Equation (32)and the four-thirds law in Equation (34).

The vertical coefficient is most easily defined, with an accepted value of $0.067hu_*$ unless density stratification restricts the value or irregular boundary geometry enhances it.

The transverse coefficient, D_y, has a standard value of $0.15hu_*$ for straight, uniform reaches. However, Ward (86), Chang (13), and others note that bends increase this to as high as $2hu_*$ if transverse velocities are not included in the equation. Prych (45) provides a means of adjusting the value of D_y to account for added spreading due to buoyancy in an initial zone. Sumer (73) notes increases of Dy in stratified flows, although the values are still below $2hu_*$.

The most difficult coefficient to evaluate is D_L, the longitudinal dispersion coefficient, which replaces D_x if averaging has occurred across the stream width. If only vertical averaging has been performed, the Elder (42) value of $D_x = 6hu_*$ is proper. It is recommended that the Holley, et al (82) method be used in conjunction with the Thatcher-Harleman (75) work for D_L in estuaries. In rivers, several methods are proposed, with the Jain (67) and Fischer (66) methods being most theoretically sound.

It has been shown that substantial distances may be required for a one-dimensional state to be reached. Equation (71) allows an estimate of the required length. It is imperative that this criterion be checked before any one-dimensional approximations are used.

SOLUTION TECHNIQUES

Both analytical and numerical solutions are reviewed. It is concluded that analytical solutions probably offer the best probable tools for the Air Force, consistent with the status of numerical models. Two exceptions are in the cases of clearly 1-D estuaries and in 2-D river systems, where existing numerical models may be very helpful.

Solutions by both the method of images and integral transform methods are discussed. Each is a powerful tool, and they provide equivalent results.

AVAILABLE MODELS

Models are presented which represent the various types of models available. It is concluded that no one model does everything, and modifications (e.g., addition of source and sink terms) are necessary to many models. In addition, some models neglect a sufficient amount of advective behavior to make coefficient selection very uncertain.

In estuaries, it is concluded that a model should include tidal velocity variation, rather than lumping it all into D_L. If the estuary can be verified as 1-D, the MIT numerical model (78) should be used. If it is not 1-D, the best available options appear to be the Yeh-Tsai (135) or Holley-Harleman (81) analytical solutions. However, questions still exist on coefficient selection, especially for the Yeh-Tsai model.

In rivers, it is preferable to use a 2-D model after vertical mixing has been achieved. The Holly (115) numerical model or the Yotsukura

and Cobb (36) analytical model both represent stream tube solutions. They incorporate channel geometry and transverse velocities. A three-dimensional model such as those by Prakash (109) and Benedict (110) are recommended for the 3-D phase prior to full vertical mixing.

RECOMMENDATIONS FOR THE FUTURE

Section VII gives a comprehensive set of recommendations relating the entire report's findings to the problem of building an effective, efficient model for Air Force planning and assessment. These will not be repeated here, but they include establishment of criteria, inclusion of velocity and geometry variations, inclusion of proper source and sink terms, model verification and documentation, and sensitivity analyses. It is believed that these recommendations point the way to development of a flexible, yet easily used model for the Air Force.

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